THERMAL PROPERTIES OF NEARLY AND WEAKLY FERROMAGNETIC FERMI SYSTEMS : SPIN FLUCTUATION EFFECTS

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CERTIFICATE

Certified that the work presented in this thesis entitled, "Thermal Properties of Nearly and Weakly Ferromagnetic Fermi Systems: Spin Fluctuation Effects", by Suresh G. Mishra has been carried out under my supervision and that this has not been submitted elsewhere for a degree.

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Thesis entitled, "Thermal Properties of Nearly and Weakly Ferromagnetic Fermi Systems: Spin Fluctuation Effects", submitted by SURESH G. MISHRA
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The present work describes a systematic study of the effect of spin fluctuations on the thermal properties of (i) nearly ferromagnetic Fermi systems, e.g. Liquid Helium 3 and (ii) weak itinerant ferromagnets, i.e. ferromagnets with a low Curie temperature ($T_c \ll T_F$). Since the real (or virtual) transition temperature in these systems is much less than T_F (the basic characteristic temperature), one is always close to a phase transition for $T \ll T_F$, and fluctuation effects are expected to be important.

The temperature dependence of the spin susceptibility χ and of the specific heat C_v of a nearly ferromagnetic Fermi system ($T_c \lesssim 0$) is usually discussed in terms of microscopic Fermi liquid theory or the paramagnon model. Results obtained in the latter calculations are valid over a very small temperature range $T < T_F \; \alpha_o$, where T_F is the degeneracy temperature of the free Fermi gas, and α_o^{-1} is the Stoner enhancement factor. One is thus unable to describe a number of significant

features of thermal properties for the degenerate range $T < T_F$. In the second and third chapters of this thesis we discuss a functional integral scheme where the Hamiltonian of a fermion system interacting via a short range two body interaction is transformed into that involving n interacting spin fluctuations ($n \geq 2$). This transformation is specially useful here because the 'fast' electronic degrees of freedom are integrated out, and the 'slow' spin fluctuation degrees of freedom are made explicit. We show that the thermal properties of this interacting spin fluctuation system can be systematically analyzed.

We analyze (in Chapter II) the contribution from one, two and three internal thermal spin fluctuations to the self energy of, say, the transverse spin fluctuation propagator (related to χ). In the low temperature regime ($T < \alpha_0 T_F$), the paramagnon theory result is reproduced; while for temperatures $\alpha_0 T_F < T < T_F$ a classical Curie like result is obtained. This latter behaviour is experimentally observed in Liq. He^3 in the corresponding temperature range. It is also shown that the spin fluctuation expansion is convergent, i.e. one need not consider the contribution of more than two internal thermal spin fluctuations to self energy. Results are compared with experimental results on Liq. He^3, good agreement being obtained with experiment for $T \lesssim 1°K$ ($T/T_F \sim 0.2$). (This work has been briefly reported in Proc. 14th Int. Conf. on Low Temp. Phys. (LT 14) Vol. 1, p. 57.)

In the third chapter $C_V(T)$ is discussed. Retaining up to the harmonic (quadratic) term of the functional Hamiltonian, one obtains the RPA for the thermodynamic potential (and hence the specific heat). If the quartic term is considered in the quasi-harmonic approximation then one can relate the thermodynamic potential to spin fluctuation propagator. Using a quasi-harmonic approximation and the experimental results for spin susceptibility, $C_V(T)_{SF}$ can be calculated. We have shown that both the Boson and Fermion contribution (c.f. E. Riedel, Z. Phys. 210, 403 (1968)) are included in our approach. We get, for $C_V(T)_{SF}$, a peaked curve with a linear rise in temperature in the low temperature side and with a slow fall on the high temperature side. In liquid He^3, for high temperatures ($\alpha_0 T_F < T < T_F$) a linear specific heat vs temperature relation is observed experimentally. The slope of C_V/R vs $\tau(=T/T_F)$ curve is $\pi^2/4$ while for a free Fermi gas the slope is $\pi^2/2$. This is accounted for by considering the suppression of density fluctuation excitations. This follows from the high sound velocity observed in Liq. He^3. A microscopic theory for this suppression is presented. A comparison of the theoretical results with experiment shows good agreement up to $\tau \lesssim 0.2$.

In the **fourth chapter**, using the above calculations, we have discussed a $T_c=0$ ferromagnet. A classical Curie

like behaviour down to 0°K is obtained. The lowest order spin fluctuation corrections are renormalizable and yield classical exponents.

The next two chapters are devoted to the magnetic phase of a weak ferromagnet ($T_c \ll T_F$). The properties discussed are magnetisation M(T) and spin wave stiffness D(T). These are usually studied in a molecular field theory (Stoner-Wohlfarth-Edwards) or in RPA (Izuyama-Kubo). These approximations seem to be quite inadequate in understanding the ferromagnetic problem as a whole, particularly at finite temperatures. A better approach has been proposed by Murata-Doniach, Moriya-Kawabata and Ramakrishnan, who discuss the effect of mode-mode coupling on thermal properties. In the fifth chapter, we have derived an expansion of free energy F in terms of the static, uniform z component ξ^z_{oo} of the spin fluctuation field ($<\xi^z_{oo}> \sim M$). Spin fluctuation effect is included in the ξ^{z2}_{oo} term. The equation for the order parameter (obtained by minimizing $F(\xi^z_{oo})$) when simplified gives an Edwards-Wohlfarth (Jour. App. Phys. 39, 1061 (1968)) like result for low temperatures ($T \ll T_c$) with a much larger coefficient for the T^2 term. Near T_c, M^2, thus obtained, decreases linearly with temperature. Spin fluctuation effects on Arrott plots are also discussed.

The penultimate chapter deals with an attempt to calculate $D(T)$ in a self consistent and spin conserving approximation which goes beyond RPA and includes spin fluctuation effects. A spin conserving approximation for the transverse spin susceptibility χ^{+-} and for the related vertex function Γ^{+-} is obtained by using Ward identity. The spin wave stiffness for small wave vectors can be obtained directly from the limiting value of a vertex $\vec{\gamma}$ which is related to Γ^{+-}. One draws a set of diagrams for $\vec{\gamma}$ and analyzes various thermal contributions. Roughly $D \propto M$. We find for low temperatures T^2 and $T^{3/2}$ terms for $D(T)$. The coefficient of T^2 term is qualitatively different from that obtained by Izuyama and Kubo. The spin fluctuation interaction or 'magnon drag' term gives $T^{5/2}$ dependence, as usual. We also show how the exchange splitting varies with temperature. (This work has been briefly presented in Mag. Letters 1, 17 (1976).)

The final chapter contains a few concluding remarks.

CHAPTER I

INTRODUCTION

eoretical study of ferromagnetism in a system of itinerant fermions started with the work of Bloch,[1] Slater[2] and Stoner.[3] Their work uses the Hartree Fock or molecular field approximation, where the two body electron-electron interaction is replaced by a self-consistently determined one body potential. In the work of Stoner,[3] the effective two body interaction is assumed to be of short range (on account of screening of the Coulomb potential by conduction electrons). The temperature dependent properties of itinerant electron ferromagnets, such as the temperature dependent spin susceptibility $\chi(T)$ in the paramagnetic phase, the Curie temperature T_c, the spontaneous magnetisation M(T) have all been discussed in the Hartree Fock approximation by Stoner, Wohlfarth[4] and others.[5] The temperature dependence of physical quantities arises in this model from the temperature dependence of the Hartree field, i.e. from the T dependence of fermion occupation numbers (Fermi Dirac distribution).

The dynamic spin susceptibility $\chi(\vec{q},\omega)$ and thence the spin wave dispersion have been considered in the RPA[6] (a level of approximation for response functions corresponding to Hartree Fock approximation (HFA) for single particle energies).

The main thrust of recent work in itinerant fermion ferromagnetism has been in more realistic treatment of the ground state (T=0 state), in particular, the effect of particle particle correlations.[7] The main qualitative conclusion of the work of Kanamori, Hubbard and Gutzwiller in this area is that the 'bare' short range repulsion U is replaced by an effective repulsion $U_{eff} < U$. This leads to more stringent conditions for the onset of ferromagnetism. The zero temperature spin wave stiffness has been calculated by Callaway and Young.[8] The temperature dependent properties can also be calculated in this approximation,[9] but one expects results qualitatively similar to that obtained in HFA, with U_{eff} replacing U.

In the mid-sixties, the role of incoherent spin fluctuations in nearly ferromagnetic fermi systems such as Liq He^3 and Pd was pointed out by Berk and Schrieffer,[10] Doniach and Engelsberg[11] and others.[12] These particle hole excitations, known as paramagnons, are the low lying excitations of the systems, and affect strongly its

temperature dependent properties. In such systems the static zero temperature spin susceptibility $\chi(T=0)$ is very large (i.e. $\chi(T=0)/\chi_{Pauli} \equiv \alpha_o^{-1} \gg 1$). It can be shown that the characteristic paramagnon energy is not T_F^o (the free gas fermi temperature) but $T_F^o\ \alpha_o \ll T_F^o$. Thus, as shown by Beal Monod et al.,[13]

$$\chi(T) = \chi(T=0) - A(T/T_F^o\ \alpha_o)^2;$$

i.e. $\chi(T)$ varies rather strongly with temperature, on a scale $T_F^o\ \alpha_o$. Because of this, the general impression has been that paramagnon theory results are valid in the rather narrow temperature range $T \ll T_F^o\ \alpha_o$.

A somewhat different aspect of spin fluctuation effects was first discussed by Doniach and Murata.[14] Using a functional intugral transformation, they showed that the Stoner Hamiltonian ($H = \sum_{k,\sigma} \epsilon_k n_{k\sigma} + U \int n_\uparrow(r)\, n_\downarrow(\vec{r})\, d\vec{r}$) could be transformed approximately into a Hamiltonian for classical interacting spin fluctuations m_q. Assuming that the number of classical spin fluctuations (i.e. those with energy $\ll k_BT$) is comparable to the number of degrees of freedom of the system, they obtained in a Hartree like approximation for fluctuations, a Curie-Weiss law for $\chi(T)$. A very different analysis by Moriya and Kawabata[15] is based on a self-consistency requirement on $\chi(\underline{q})$. They assume that the RPA expression for $\chi(\underline{q})^{-1}$ is modified by an additive

constant. This constant is determined by requiring that the susceptibility satisfies the identity $\chi = (\partial^2 F_M/\partial M^2)_{M\to 0}$, the free energy being determined as the sum of ladder and bubble diagrams. This work also established that near T_c, the number of thermal spin fluctuations is equal to N (number of degrees of freedom of the system) x $(T/T_F^o)^{1/3}$. Moriya, Kawabata and coworkers[16] have since then discussed spin fluctuation effects in magnetisation, spin lattice relaxation time, in itinerant electron antiferromagnets. There is experimental evidence for the effects calculated.[17] Ramakrishnan[18] attempted to discuss spin fluctuation effects from first principles, starting from an equation of motion for $\chi(\vec{q},w)$ which leads to a three particle Green's function G^{III}, making a diagrammatic interacting spin fluctuation analysis of the latter. He showed how spin fluctuation effects could be decomposed into zero point and thermal parts. Further he found that the coupling constants, such as the critical coupling for ferromagnetism, and the four fluctuation coupling constant were likely to be very different from their zeroth order value because of the intermediate coupling nature of the problem. He further estimated fluctuation correlation effects which, very close to T_c, dominate the mean fluctuation field term (responsible for a Curie-Weiss law). More recent papers on the subject are due to Hertz and

Klenin,[19] Murata,[20] Kawabata,[21] Yamada,[22] Hertz,[23] Gumbs and Griffin.[24]

Inspite of the large amount of work in this area, there has been no systematic attempt to discuss spin fluctuation effects in nearly and weakly ferromagnetic fermi systems from first principles. We try to do this in the present work.

The area of our concern can be described by the parameter space of Fig. 1, where the x axis represents the short range interaction U in the units of $\rho_{\varepsilon_F}^{-1}$. The y axis is temperature $k_B T$ in the same units. The fermion system has a paramagnetic ground state for small U, and presumably (i.e. if it is not a Mott-Hubbard insulator, antiferromagnet) a ferromagnetic ground state for large U. The boundary is located at $U\rho_{\varepsilon_F} = 1$ in HFA. Earlier work on correlation effects can be viewed as an attempt to rescale the x axis, i.e. to find $U_{eff}\ (U, \rho_\varepsilon)$ and to locate the point $U_{eff}\ \rho_{\varepsilon_F} = 1$. Starting from this point, a curve can be drawn in the (T,U) plane, separating the paramagnetic and ferromagnetic phases. Close to $U\rho_{\varepsilon_F} = 1$, the curve (marked SW) is parabolic in the HFA, i.e. $(T_c\ \rho_{\varepsilon_f})^2\ \alpha\ (U\rho_{\varepsilon_F}-1)$. This follows simply from the nature of the degenerate fermi distribution. In the work of Moriya et al. this is replaced by a nearly straight line marked MDMK. Consider

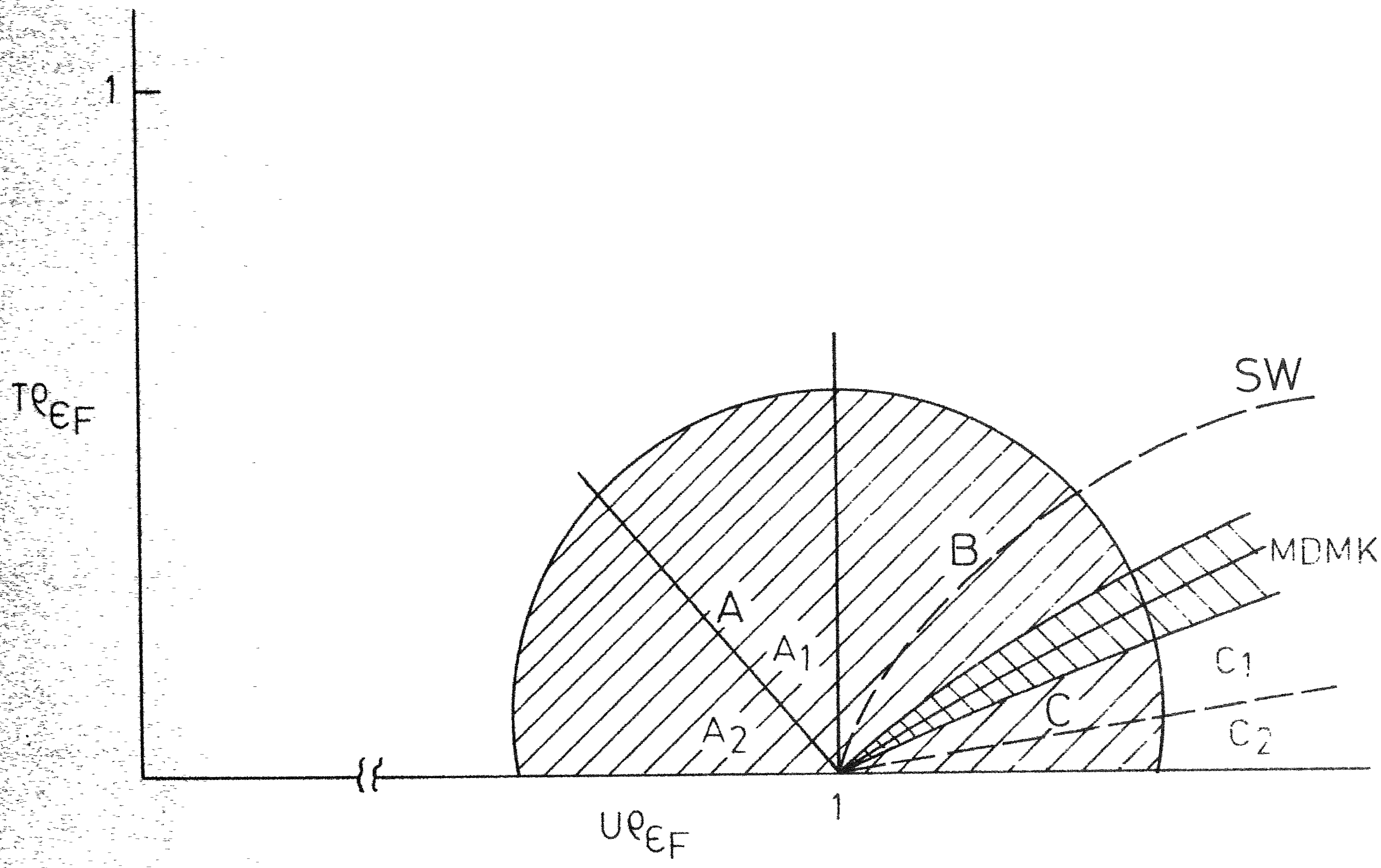


Fig. 1. $U\rho_{\epsilon_F}$, τ space for near and weak ferromagnets

the shaded region $|U\rho_{\varepsilon_F}-1| << 1$, $T\rho_{\varepsilon_F} << 1$. The system is always degenerate, and since (for $U\rho_{\varepsilon_F} \gtrsim 1$) m_0^2 (saturation magnetization at T=0, in dimensionless units) $\alpha\,(U\rho_{\varepsilon_F}-1) << 1$, magnetic ordering affects electronic energies only weakly. Clearly, in this region, one is always close to the ferromagnetic instability. Thus longitudinal and transverse spin fluctuation excitations always have characteristic energies much lower than $\rho_{\varepsilon_F}^{-1}$, so that the temperature dependent properties are expected to be dominated by these excitations.

The nearly ferromagnetic regime is the region A, bounded by the line $U\rho_{\varepsilon_F}=1$. In the area close to $k_B T\rho_{\varepsilon_F}=0$, i.e. in the lower half A_2 (bounded by $T\rho_{\varepsilon_F} \simeq (1-U\rho_{\varepsilon_F})$) lies the 'paramagnon' regime. In the part A_1 one is probably in a classical spin fluctuation region, as is also plausible from its contiguity with B, the paramagnetic regime, where classical spin fluctuations dominate the temperature dependent properties. The weakly ferromagnetic region C is also divisible broadly into a 'classical' regime C_1 close to the transition line and a region C_2 analogous (in its characteristic temperature dependence) to the 'paramagnon' regime A_2.

In this thesis, we first consider the region A. We show how the Hamiltonian of the system can be transformed into that involving n interacting spin fluctuations ($n \geq 3$).

The transformation maintains rotational invariance and no 'classical' or zero frequency approximation is made. The fast electronic degrees of freedom are integrated out, and determine the s.f. coupling. We first consider the $\chi(T)$ of this interacting s.f. system, and analyze the contribution from one two and three internal s.f.s to the self energy Σ of say the transverse s.f. propagator (related directly to χ). Such a spin fluctuation interaction expansion is shown to be convergent; i.e. the leading terms in Σ involve one and two correlated internal s.f.s. The three s.f. contribution is less by at least one power of $T\rho_{\epsilon_F}$ (see Chapter II for details). Further, it is seen that the same physical process (diagram) is called the paramagnon process in the low temperature or A_2 regime and classical s.f. in A_1. One thus obtains in a single scheme, a theoretical expression for $\chi(T)$ which gives the leading term for the entire region A. We compare our prediction with experimental results[25] for $\chi(T)$ of liquid He^3. He^3 is a pure homogeneous fermi liquid, and thus is free of unknown complicating effects due to band structure (density of state structure) present in nearly magnetic metals. Further, by increasing pressure, one can come quite close to the boundary $U\rho_{\epsilon_F}=1$. We find very good agreement with experiment, over a temperature range $0.0 < \tau = T\rho_{\epsilon_F} < 0.2$.

We then study (in Chapter III) the thermal properties of a nearly ferromagnetic fermi system, and calculate the specific heat in an approximation which is shown to retain the leading term. Again comparison is made with liquid He^3, for which $C_V(T)$ data are available. Good agreement with experiment is obtained over a temperature range $0 \leq \tau \leq 0.2$. The shape of the $C_V(T)$ curve showing a low temperature bump and a linear flattening out $C_V(T) \simeq \frac{\pi^2}{4}\frac{T}{T_F^o}$ (i.e. half the free fermi gas value) are both explained. The former is due to spin fluctuations and the latter to the fact that density fluctuation excitations have a high characteristic energy (compressibility $\sim$1/10 of free fermi gas compressibility).

We believe that the very good agreement between theory and experiment over a broad temperature region argues strongly for the quantitative correctness of our systematic theory, since He^3 is a very clean case. Supporting evidence is present in the experimental $\chi(T)$ values of various nearly ferromagnetic metals and alloys, e.g. Ni_3Ga, $HfZn_2$, NiRh, Pd, YCo_2, U_2C_3 etc. Their $\chi(T)$ curve is quite similar to that discussed above for He^3.

The region B, i.e. the paramagnetic region, has been investigated by several authors, as mentioned above. Here, the one and two internal s.f. approximation for Σ becomes insufficient close to T_c. An estimate of the three s.f.

contribution, made by Ramakrishnan,[18] can be used to roughly demarcate the critical region (Fig. 1, shaded area close to the line MDMK). An interesting point is the shrinkage of the critical region as $T_c \to 0$. In particular, a $T_c=0$ ferromagnet is expected to have purely classical (mean field) critical indices. This has also been pointed out recently by Hertz[23] using a renormalization group method. In Chapter IV, we present explicit calculation for $\chi(T)$, confirming this expectation.

The remainder of the thesis is devoted to the region C, i.e. the ferromagnetically ordered phase of a weak ferromagnet ($m_o^2 \ll 1$ or $T_c\, \rho_{\varepsilon_F} \ll 1$). We obtain an equation for $m(T)^2$ in an approximation scheme retaining the leading thermal spin fluctuation effect. We find that $m(T)^2$ is strongly coupled to spin fluctuations. Longitudinal spin fluctuations have low characteristic energies $m^2\varepsilon_F$. The transverse spin fluctuation spectrum has a low lying spin wave pole at frequencies $\omega_q=Dq^2$ ($D \propto m$, roughly) and has a resonance structure in the Stoner continuum. We calculate the spectrum of these fluctuations and find their effect on m^2. The effect is seen to determine its temperature dependence; that arising from temperature dependence of the fermi distribution is very weak. At low temperatures ($T\,\rho_{\varepsilon_F} \ll m^2$), we find $m^2(T)=m_o^2\left(1-A\,\frac{(T\,\rho_{\varepsilon_F})^2}{m_o^4}\right)$

where A is a constant. The spin wave contribution to $m^2(T)$ is smaller by a factor m_o. This is in accord with experiment. Well above $T_c/2$, the T^2 dependence changes to a classical form $m^2 \propto (T_c-T)$. We do not attempt a detailed comparison between experiment and theory for obvious reasons. However, the study of magnetisation $M(H,T)$ in a magnetic field H provides a case where a qualitative new prediction can be made. Here, Wohlfarth et al.[26] have shown, by analyzing a Ginzburg Landau like model with a Stoner-Wohlfarth temperature dependence for $M(T)$, that the Arrott plot of $M^2(H,T)$ against $H/M(H,T)$ should be a straight line. The same paper exhibits Arrott plots for NiPt alloys; these are systematically and decidedly curved for small H/M. We obtain the Arrott plot expression in an approximation scheme retaining spin fluctuation effects. We show that the deviation from linearity can be qualitatively explained for small H/M and large temperatures.

In Chapter VI, we take up the question of the temperature dependence of the spin wave stiffness D in a weak ferromagnet. In the RPA,[6] $D(T) \propto m(T)$ for small m; this m being the spontaneous magnetisation in the HFA. Beyond the RPA, there are very few results. A general phenomenological analysis due to Izuyama and Kubo[27] leads to the low temperature form

$$D(T) = D(T{=}0) - AT^{5/2} - BT^2,$$

the coefficients A and B being unknown. This is also confirmed by the microscopic analysis of de Pasquale and Corrias[28] for a strong ferromagnet ($N_\uparrow = N$, $N_\downarrow = 0$). We are interested in knowing whether and how the spin fluctuation excitations affect D(T). For this purpose, we start from an approximation for electron self-energy Σ_e which includes the effect of electron scattering from spin fluctuations. Then, by following a standard method, we construct a spin conserving approximation for the transverse or spin flip response function. From this we determine the spin wave stiffness D. We find that at low temperatures

$$D(T) = D_o\,(1 - A'\,T^{3/2} - B'T^2),$$

i.e. there is a $T^{3/2}$ term due to transverse spin fluctuation (spin wave) contribution to single particle self-energy, and a T^2 term arising from longitudinal and incoherent transverse spin fluctuations. The size of the $T^{3/2}$ term, however, is smaller than that of the T^2 term by a factor m. There are no experiments on D(T) in weak ferromagnets, to compare with our prediction. However, large T^2 terms are reported for D(T) in many itinerant electron ferromagnets.[29]

In the concluding chapter, we point out a few areas where further work is needed, and also other phase transitions in fermi system where such fluctuation effects might be significant.

SPIN SUSCEPTIBILITY

1. Introduction

In this chapter we address ourselves to the problem of the temperature dependence of spin susceptibility $\chi(T)$ of nearly ferromagnetic fermi systems.[30] These systems are characterised by an enhanced zero temperature susceptibility. An ideal example of such a system is normal liquid helium-3.[31] There are some metals, e.g. palladium[32] and alloys like Ni_3Ga,[33] $HfZn_2$,[34] U_2C_3,[35] YCo_2,[36] NiRh[37] which also show such behaviour. In the calculation we will refer to liq. He^3 only, as there are no band structure and density of states complications. We can, therefore, work in the parabolic band model $\varepsilon_k = \hbar^2 k^2/2m$ and with free fermi gas density of state, $\rho(\varepsilon)$.

The most recent and precise experimental work on $\chi(T)$ of Liq He^3 is by J. R. Thompson[25] and his associates at Duke University. The work reveals two characteristic features in two different temperature regimes.

(i) At very low temperatures the data can be represented by the expression

$$\chi(T) = \frac{\chi_P}{\alpha_o} \{1 - 3 (\frac{T}{T_F^o \alpha_o})^2\} \quad (1.1)$$

This doubly enhanced T^2 dependence has been predicted by paramagnon theory, but the observed behaviour is over a wider (τ^2 behaviour even for $\tau \sim \alpha_o$) temperature range.

(ii) At sufficiently high temperatures (T > 0.5°K) the susceptibility is found to tend asymptotically towards the Curie law relation, with a large Curie constant. Note that though the system is highly degenerate ($T << T_F^o$), its magnetic behaviour is like that of a collection of independent classical moments. This is surprising.

A good microscopic theory should explain these features, at least qualitatively. We direct our effort to attain this goal. Before doing that, let us pause for a while and review earlier attempts in this direction.

There are several theories with which the experiments in temperature range T << 0.5°K can be compared. For an ideal fermi gas with a degeneracy temperature $T_F^o = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}/k_B$, the susceptibility χ_{id} can be represented, for $\tau \leq 0.1$ by the expression

$$\chi_{id} = \chi_P \left(1 - \frac{\pi^2}{12} \tau^2 + \ldots\right) \quad (1.2)$$

For Liq He^3 the effect of interaction between spins has the effect of increasing χ_o over the expected value by a factor vary

between 10 and 20 according to the density. The Stoner theory[3] for a fermi gas with interaction then predicts $\chi^{-1} = \chi_{id}^{-1} - U$, U is the density dependent quantity proportional to the exchange integral. Assuming U to be temperature independent, one obtains in the low temperature limit

$$\chi(T) = \frac{\chi_p}{\alpha_o} \{1 - \frac{\pi^2}{12} \frac{\tau^2}{\alpha_o} + \ldots\} , \qquad (1.3)$$

a singly enhanced τ^2 dependence. The next attempt was that due to Richards[38] who calculated lowest order temperature corrections to fermi liquid theory result and expressed the coefficient of T^2 term as function of certain parameters obtained from a combination of specific heat and susceptibility results.

The most remarkable result is due to Beal Monod[13] et al., who calculated $\chi(T)$ near T=0°K in the paramagnon model. They calculated the correction to free energy due to transverse and longitudinal paramagnons (or spin fluctuations) represented by a collection of ladder and ring diagrams respectively. The corresponding correction to zero temperature susceptibility is found for $\tau << \alpha_o$ to be

$$\chi(T) = \frac{\chi_p}{\alpha_o} \{1 - \frac{3.2\pi^2}{24} (\frac{\tau}{\alpha_o})^2 + 0 \{(\tau/\alpha_o)^4 \ln (\tau/\alpha_o)\}\} \qquad (1.4)$$

There is no adjustable parameter introduced and the magnitude of the third term is small in comparison to the second

one for $\tau << \alpha_0^{3/2}$. Also notice that there is no $T^2 \ln T$ term in the susceptibility. (Such a term is obtained by Barnea[39] and Misawa.[40]) The theory works quite well in the low temperature regime. It appears as though the theoretical expansion parameter is (τ/α_0) whereas the form (2.1.4) seems to represent experimental results accurately up to $\tau/\alpha_0 \approx 0.3$(?). This approach is also marred by a lack of self consistency, first pointed out for itinerant electron ferromagnetism by Moriya and Kawabata.[15]

In the region of 0.5°K and above where the susceptibility tends towards the classical Curie like behaviour, the theoretical prediction of $\chi(T)$ is a difficult problem because the thermal energy $k_B T$ is higher than spin fluctuation energy $\alpha_0 \, \varepsilon_F$ and lower than the fermi energy $k_B T_F$ and the interaction energy U. The Murata-Doniach approach involving classical interacting spin fluctuations, has been successful in predicting a Curie-Weiss law for $\chi(T)$ for magnetic systems $(T > T_c)$.

However, so far there exists no microscopic theory applicable over the entire temperature range, i.e. one which describes accurately both the paramagnon behaviour and the 'classical' behaviour, as well as the intermediate region, with well defined limits of validity and accuracy. We consider, in this chapter, a microscopic spin fluctuation

theory and show that it is possible to understand the temperature dependence of $\chi^{-1}(T)$ over a wide temperature range $\tau << 1$ (but not necessarily $\tau/\alpha_o << 1$). The leading terms are then used to calculate $\chi^{-1}(T)$ for He^3, for $\tau \lesssim 0.2$. The agreement with experiment is good, and the deviation at high τ explicable as to size and sign. We summarize our theory now, details being given in succeeding sections.

Obviously, the low lying ($|\vec{q}| << k_f, \omega << \varepsilon_f$) spin fluctuations (paramagnons) are important in determining the low temperature ($\tau << \alpha_o$) behaviour of the system. Their effect dominates over that due to uncorrelated or 'free' particle hole (Stoner) excitations because of the exchange enhancement. It is suggested that if the effect of interaction between spin fluctuations is calculated self consistently (mean fluctuation field approximation, MFFA), one may get a qualitative understanding of the behaviour in the high temperature ($\tau >> \alpha_o$ but $\tau << 1$) regime also. In the functional integration scheme, on taking the trace over the fermion variables, we have an effective interacting spin fluctuation Hamiltonian $F(\vec{\xi}_{q,u})$, with n spin fluctuation coupling ($n \geq 3$). The 'bare' coupling constants can be evaluated in terms of the free fermi gas parameters and depend mildly on momentum ($q/2k_f$), energy (ω/ε_f). The fluctuation propagator

$$D^{\alpha\beta}(\vec{q}, z_m) = \int_0^\beta \langle T\ (\xi^\alpha_{\vec{q}u}\ \xi^\beta_{\vec{q}o})\rangle e^{-uz_m}\, du, \tag{1.5}$$

is directly proportional to the spin susceptibility function $\chi^{\alpha\beta}(\vec{q}, z_m)$ of the system We therefore analyze D. The bare fluctuation propagator D_o corresponds to RPA. We are interested in the temperature dependent contributions to D ($D^{-1} = D_o^{-1} - \Sigma$). These can be isolated in principle by performing the frequency sums in diagrams for Σ, and considering terms with one or more positive frequency Bose parts (i.e. $\theta(\omega)\ (\exp(\beta\omega) - 1)^{-1}$). Introduction of one internal spin fluctuation line in Σ leads to the equation[30]

$$\chi(\underline{q})\ \chi^{o}(\underline{q})^{-1} = (1 - U_{eff}\,\chi(\underline{q}) - \lambda \sum_{\underline{q}'} \chi(\underline{q}'))^{-1} \qquad (1.6)$$

for susceptibility. The renormalized four fluctuation coupling vertex $\lambda_{\underline{q}'}$ cannot be evaluated reliably. Because of its mild dependence on ω, q and T, we approximate it by a constant λ. Contribution from incoherent fluctuation terms and zero point (T=0) part of λ term are lumped together and are assumed to renormalize U (to U_{eff}). For $\tau << \alpha_o$, the equation (1.6) need not be solved self consistently and one has the paramagnon theory result: $\Delta(\chi^{-1}) \propto \tau^2/\alpha_o$. For temperatures $\alpha_o < \tau << 1$, the self consistent solution leads to a Curie like behaviour: $(\chi^{-1}) \propto \tau$.

The above expression for χ is useful if correction terms are small. The next thermal correction terms for Σ are due to two and three internal, correlated spin fluctuations

Qualitatively, the contribution of Σ^{II} (correlated) is similar to one s.f. term. The resulting contribution to $\chi^{-1}\chi_p$ from Σ^{III} is estimated to be less than $\tau^4 \alpha_o^{-3}$ for $\tau < \alpha_o$ and thus very small. For $\tau << 1$ but $\tau \geq \alpha_o$, the estimate is $\tau^2 \ln(1/\alpha)$. The mean particle field term goes as τ^2. Thus these corrections are of relative order τ, and the solution of the above equation is expected to give a correct $\chi(T)$ for $\tau << 1$. This smallness of correlation effects is due to only a small fraction of the total degrees of freedom being excited since $T << T_F^o$.

We have made a detailed calculation of the susceptibility of Liq He^3, using equation (2.1.6) plus Σ^{II} corrections also included. The agreement is very good up to $\tau = 0.2$ and becomes progressively poorer. The fluctuation correlation correction is of the correct sign and size to explain the difference between theory and experiment.

To summarize, we have a scheme where the effect of one, two and higher thermal spin fluctuation can be calculated systematically from the first principles. We have shown that if the paramagnon effects are calculated self consistently, one can understand the temperature dependence of spin susceptibility over a wide range of temperature.

In the following sections we derive the functional Hamiltonian and calculate the effect of one, two and three internal, correlated thermal spin fluctuations. Then we compare our results with the previous theories and the experimental results on Liq He^3 and other metals and alloys. The calculations and analysis presented in this chapter are rather detailed and will be referred to quite frequently in the subsequent chapters.

2. Fluctuation Interaction Theory

It is possible to transform the basic Hamiltonian of the system, given in terms of the Fermion variables, to an effective Hamiltonian expressed as a power series in interacting fluctuation fields (Boson variables). This is done by using the well known method of functional integration.[41-46] The result is that the slow spin fluctuation degrees of freedom are made explicit, their 'bare' spectrum and the coupling between them being determined by a trace over the fast electronic degrees of freedom. Clearly the transformation is particularly useful if $\omega_{slow} \ll \omega_{fast}$. In our case this translates into $T_c \ll T_F$ for the weakly ferromagnetic case and $\chi(T=0)^{-1} \ll \chi_{Pauli}^{-1}$ for the nearly ferromagnetic case. We analyze the effect of some lowest order terms in such expansions.

2a. Functional Integral Formalism

Let us start by discussing the functional integral formulation of the theory of itinerant Fermion systems. The rules for such a transformation have been given by Rice.[45] We simply transcribe them for our case. Here the statistical operator is represented as a functional integral (a Gaussian functional average) over a 'time' ordered exponential. Feynman time ordering is necessary when different terms in the Hamiltonian (in the exponential) do not commute with each other.

The Hamiltonian of an interacting fermion system is given by

$$H - \mu N = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} \, a^{\dagger}_{\vec{k}} \, a_{\vec{k}} + V \sum_{\vec{q}} \rho_{\vec{q}} \, \rho_{\vec{q}} - U \sum_{\vec{q}} \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}} \qquad (2a.1)$$

For detailed discussion about this form the appendix I may be referred. Here $a_{\vec{k}}$ and $a^{\dagger}_{\vec{k}\sigma}$ are annihilation and creation operators for fermions of momentum $\vec{k}$ and spin σ. $\varepsilon_{\vec{k}}$ is the single particle energy measured from the chemical potential μ. $\rho_{\vec{q}}$ and $\vec{S}_{\vec{q}}$ are Fourier transforms of number density and spin density operators respectively. We have written the interaction in a form which is explicitly invariant under rotations. An effective zero range interaction between the fermions is parametrized by V and U which can be related to experimental properties through dynamical models.

The grand partition function is defined by

$$Z = e^{-\beta\Omega} = \mathrm{tr}\ \exp\ [-\ \beta(H-\ \mu N)]\ , \qquad (2a.2)$$

where $\beta = 1/k_B T$. Substituting $H-\mu N$ from the equation (2a.1) and introducing an ordering label s, we write

$$Z = \mathrm{tr}\ \exp\left\{ -\frac{\beta}{N}\ \left[\sum_{k\sigma s} \epsilon_k\ a^\dagger_{k\sigma s}\ a_{k\sigma s} + V \sum_{qs} \rho_{qs}\ \rho_{-qs} - U \sum_{qs} \vec{S}_{qs} \cdot \vec{S}_{-qs} \right]\right\} \qquad (2a.3)$$

The sum over s runs from 1 to N. With the introduction of the ordering label, the operators in the exponent can be treated as c numbers with an error which goes to zero as $N \to \infty$. Using the Stratonovich-Hubbard identity,

$$\exp\ \{|a|^2\} = \int_{-\infty}^{\infty} \frac{dx_1 dx_2}{\pi} \exp\ \{-\ |x|^2 + ax^* + a^*x\} \qquad (2a.4)$$

where $x = x_1 + ix_2$ etc., one can express the partition function as a functional integral over Boson variables f, $\vec{\xi}$;

$$Z = \int_{-\infty}^{\infty} \prod_{q,s,i=1,2} \left\{ \frac{df_{qsi}}{\pi\sqrt{N}}\ \frac{d\vec{\xi}_{qsi}}{\pi^3\ \sqrt{N}^3} \right\}$$

$$\exp\ \left\{-\ \frac{1}{N} \sum_{qs,\,j=1,3} (|f_{qs}|^2 + |\vec{\xi}_{qsj}|^2)\right\} \times$$

$$\times L\ \{f_{qs},\ \vec{\xi}_{qs}\} \qquad (2a.5)$$

where

$$L\ [f_{qs},\ \vec{\xi}_{qs}] = \mathrm{tr}\ \exp\ \left\{-\ \frac{\beta}{N}\ \left[\sum_{k\sigma s} \epsilon_k\ a^\dagger_{k\sigma s}\ a_{k\sigma s} - \sum_{qs} c^\rho (\ \rho_{qs}\ f^*_{qs} + \mathrm{h.c.}) - \sum_{qsj} c^s (S^j_{qs}\ \xi^j_{qs}{}^* + \mathrm{h.c.})\right]\right\}$$

$$j = z,\ +,\ -. \qquad (2a.6)$$

$$\text{with} \quad c^{\rho} = \left(-\frac{V}{\beta}\right)^{1/2}, \quad c^{s} = \left(\frac{U}{\beta}\right)^{1/2}. \tag{2a.7}$$

Here L behaves like the partition function of a system of non-interacting fermions moving in presence of a set of random time dependent fields. As $N \to \infty$, the set of points $\{\vec{\xi}_s\}$ etc., becomes a continuous function $\vec{\xi}(u)$ defined on the interval $[0,\beta]$ with the boundary condition $\vec{\xi}(0) = \vec{\xi}(\beta)$ etc. and $\beta/N \sum_s \to \int_0^\beta du$. The above condition originates from the boundary conditions imposed on Green's function and operators in the imaginary time domain. Now the quantities depending on u can be expanded in a Fourier series as is usually done in finite temperature many body theory, and Eqn. (2a.5) becomes,

$$Z = \int \prod_{\alpha, i} \frac{df_\alpha \, d\vec{\xi}_{\alpha i}}{\pi^4} \exp\left(-\sum_\alpha \left(|f_\alpha|^2 + |\xi^z_\alpha|^2 + |\xi^+_\alpha|^2 + |\xi^-_\alpha|^2\right)\right)$$

$$L\{f_\alpha, \xi^z_\alpha, \xi^+_\alpha, \xi^-_\alpha\} \tag{2a.8}$$

where $\alpha = (\vec{q}, z_m)$ and m runs over all integers and

$$L\{f_\alpha, \vec{\xi}_\alpha\} = \mathrm{tr}\, T_u \exp\{-\int_0^\beta du \sum_{k\sigma} \varepsilon_k a^\dagger_{k\sigma}(u) \, a_{k\sigma}(u)$$

$$+ c^\rho \frac{1}{\beta} \int_0^\beta du \sum_\alpha (f^*_\alpha \, \rho^\dagger_{qu} \, e^{2\pi imu/\beta} + \text{h.c.})$$

$$+ c^z \frac{1}{\beta} \int_0^\beta du \sum_\alpha (\xi^{z*} \, S^z_{qu} \, e^{2\pi imu/\beta} + \text{h.c.})$$

$$+ c^+ \frac{1}{\beta} \int_0^\beta du \sum_\alpha (\xi^{+*} \, S^+_{qu} \, e^{2\pi imu/\beta} + \text{h.c.})$$

$$+ c^- \frac{1}{\beta} \int_0^\beta du \sum_\alpha (\xi^{-*} \, S^-_{qu} \, e^{2\pi imu/\beta} + \text{h.c.})\} \tag{2a.9}$$

to expand $Y[f,\vec{\xi}]$ in powers of the fields, i.e.

$$Y[f,\vec{\xi}] = \sum_{\vec{q},m} K_2(q,m)|f_{qm}|^2 + \sum_{\vec{q}_i,m_i} K_4(\vec{q}_1,m_1;\vec{q}_2,m_2;\vec{q}_3,m_3;\vec{q}_4,m_4)$$
$$f(\vec{q}_1 m_1)\ f(\vec{q}_2 m_2)\ f(\vec{q}_3,m_3)\ f(\vec{q}_4,m_4)\ \delta(\sum_{i=1}^{4}\vec{q}_i)\ \ (\sum_{i=1}^{4} m_i) + \ldots$$
$$+ \sum_{\vec{q}m} G_2^{\alpha\beta}\ (\vec{q},m)\ \ |\vec{\xi}_{qm}|^2 + \sum_{\vec{q}_i,m_i} G_4^{\alpha\beta\gamma\delta}(\vec{q}_1 m_1;\vec{q}_2 m_2;\vec{q}_3 m_3;\vec{q}_4 m_4)$$
$$\xi_{\alpha}(\vec{q}_1 m_1)\ \ \xi_{\beta}(\vec{q}_2 m_2)\ \ \xi_{\gamma}(\vec{q}_3 m_3)\ \ \xi_{\delta}(\vec{q}_4 m_4)\ \delta(\sum_{i=1}^{4} q_i)\delta(\sum_{i=1}^{4} m_1)$$

$+ \ldots. +$ terms involving coupling between spin and density fluctuations; (2a.13)

where $\alpha, \beta, \gamma, \delta$ are the spin indices. The coefficients K's and G's are given in terms of closed fermion loops. For example,

$$G_2^{\alpha\beta}\ (q,m) = (1 - U\ \ \chi_o^{\alpha\beta}(q,m))$$

where χ_o is the functional evaluated by Lindhard for a free fermion model. In the interacting fluctuation fields, these coefficients can be regarded as the vertices.

Clearly the form is analogous to that discused by Ginzburg, Landau and Wilson for classical interacting fluctuation fields. The quantum effects can be traced to the non-commutativity of H_o and H', which force us to write $\exp(-\beta H)$ in the interaction representation, requiring the functional averaging identity (2a.4) to be applied for each time u. This makes the order parameter time dependent, with the consequence that (Matsubara) frequencies (z_m) appear on the same footing as wave vectors.

Now we can write the interacting fluctuation Hamiltonian in a physically motivated approximation scheme and carry out the functional averaging. This gives the partition function and hence the thermal properties. In the next chapter we will use this procedure to calculate the specific heat of Liq He^3. Here we consider the magnetic susceptibility and its temperature dependence. From the expression for $Y[f,\vec{\xi}]$ it is seen that the thermal properties are determined by the density fluctuations, the spin fluctuations and their interactions. Since the contribution of the interaction of density fluctuation and longitudinal spin fluctuations to $\chi(T)$ is quite small, we neglect it.

An expression for the static spin susceptibility which is defined as

$$\chi(0) = -\frac{1}{\beta} \left. \frac{\partial^2 \ln Z}{\partial h^2} \right|_{h \to 0} , \qquad (2a.14)$$

can be written in terms of the functional average. As the field h enters additively with ξ^z_{oo} in Z, a simple change of variables from ξ^z_{oo} to $\xi^z_{oo} - \frac{g\mu_B h}{c^z}$ yields the expression

$$\chi(0,0) = \frac{(g^2 \mu_B^2)}{U} [2 < \xi^{z^2}_{oo} > - 1] \qquad (2a.15)$$

where < > denotes the functional average. The above result can be generalized to that for the dynamical susceptibility

$$\chi^{\alpha\beta}(q, z_m) = g^2 \mu_B^2 \frac{1}{U} [D^{\alpha\beta}(\vec{q}, z_m) - 1] \qquad (2a.16)$$

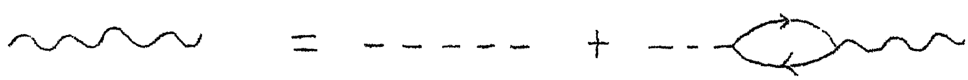
where $D^{\alpha\beta}(\vec{q}, z_m)$ is the fluctuation 'propagator'. Thus to calculate the response of the system we have to calculate the averages $\langle|\xi_q^z|^2\rangle$ and $\langle|\xi_q^+|^2\rangle$, etc.

2.2b Spin Fluctuation Expansion

The fluctuation propagator D can be obtained from $Y[\vec{\xi}]$, using the diagrammatic rules given in Appendix II. The bare propagator is, as usual, the inverse of the coefficient of the quadratic term in the Hamiltonian,

$$D_o^{-1} = [1 - U\chi^o(\underline{q})] \tag{2b.1}$$

Denoting the totally free fluctuation propagator ($U=0$) by a dotted line, ---, the above equation can be expressed as



(2b.2)

where the wavy line represents the propagator D_o, and the continuous lines are fermion propagators. This approximation, where no fluctuation interaction effects are included, is the RPA.[6]

The lowest order self energy diagrams for the transverse s.f. propagator which result on including the quartic interaction effects are shown in Figs. 2a to 2c. The propagator D is given in terms of Σ by the Dyson equation

$$D^{-1} = D_o^{-1} - \Sigma \tag{2b.3}$$

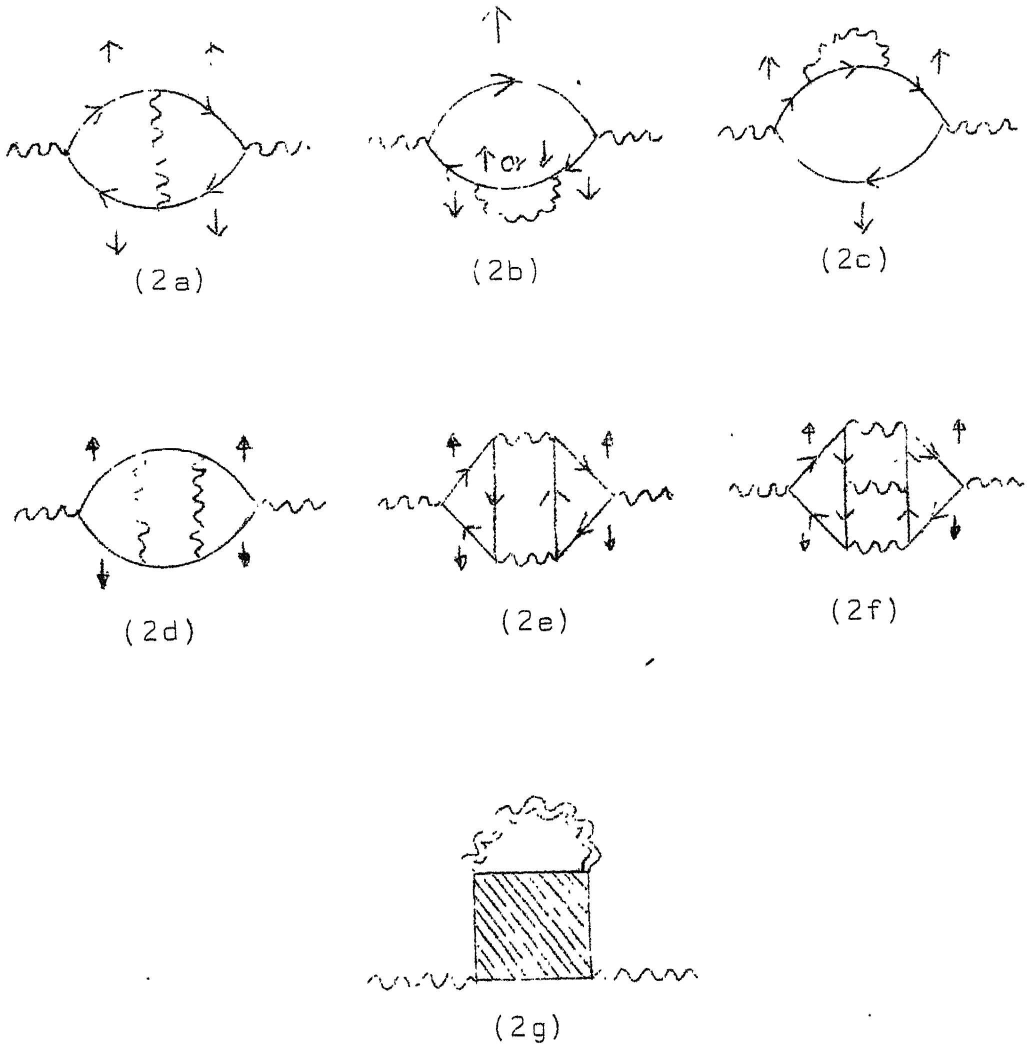


Fig. 2. Self energy diagrams for the transverse spin fluctuation propagator.

Higher order diagrams are shown in Figs. 2d to 2f. Now we systematically analyse the temperature dependence of the contribution due to these diagrams.

The temperature dependence of $\Sigma(q = 0, m = 0)$ arises from internal frequency summations which can be connected to integrations over frequency with a Bose factor, i.e. to $\int_{-\infty}^{\infty} \phi(\omega, T) (\exp (\beta\omega)-1)^{-1}$. This can be divided into a zero point part and a thermal part. The former is non zero at zero temperature and depends very weakly on temperature through the explicit temperature dependence of $\int_{-\infty}^{\infty} \phi(\omega, T) d\omega$. This function depends explicitly upon the fermion variables only and can be shown to be characteristically of the form $A + B\ (T/T_F^o)^2$ at low temperatures. We omit such terms. The thermal contribution is expected to be sizeable if there are considerable low energy fluctuations, and if their coupling is strong. The former is true near a ferromagnetic instability and the latter is true in our case because the coupling is via electrons. Thus the coupling has a size U, range $\sim 2k_f$ and ϵ_f in wave vector and energy space respectively.

Consider first the thermal part of the diagram (Fig. 2a). Its contribution to Σ is

$$\Sigma^{2a} (0,0) \sim \sum_q G_{p\uparrow} G_{p+q\uparrow} D_q^o\ G_{p\downarrow} G_{p+q\downarrow} . \tag{2b.4}$$

If the system is nearly ferromagnetic, $D^{-1}(0,0) << 1$, one should use D rather than D^o in such diagrams, i.e. work

with skeleton diagrams. It is difficult to calculate Σ^{2a} exactly. Nevertheless, since D is peaked for small $\vec{q}$ and ω, one can expand the fermion propagator functions in powers of $(\vec{q},\omega)$. The $|\vec{q}|=0$, $\omega=0$ part of such an expansion gives the leading temperature dependence. The leading (q^2 or ω^2) corrections give, in the paramagnon limit, ($\tau << \alpha_o$) a contribution of relative order τ^2 and in the classical limit a contribution of relative order $\tau^{2/3}$ and hence are small since $\tau<<1$. This physically amounts to assuming that the coupling between low frequency ($\omega \leq k_B T$), long wave length ($q < \sqrt{\alpha_o}\, k_f$ or $k_f(k_B T/\varepsilon_f)^{1/3}$) spin fluctuations is of zero range in space and time (constant in $\vec{q},\omega$ space). Actually, the time of interaction is ε_f^{-1} and is much shorter than typical ω_{sf}. The same is true for the length scale ($q^{-1}_{s.f.} >> (2k_f)^{-1}$). One can now compact the diagrams 2a-2c into a single term where the value of the effectively zero range instantaneous coupling can be evaluated through Figs. 2a-2c. It is clear that this coupling depends on temperature in the scale $(T/T_F^o)^2$ and thus the temperature dependence is weak.

The contribution of Fig. 2g to the fluctuation self energy is

$$\Sigma^{I}(0,0) = -\lambda \frac{1}{\beta\Omega}\sum_{\underline{q}} D\,(\underline{q}) \,. \tag{2b.5}$$

In the paramagnetic phase the contribution is the same for longitudinal as well as transverse spin fluctuations. One thus has up to this order,

$$D(\underset{\sim}{q}=0) = (1- U\chi(0) - \Sigma^{I}(0))^{-1}$$
$$= (1- U\chi(0) - \Sigma^{I}_{T=0}(0) - \Sigma^{I}_{T}(0))^{-1} . \qquad (2b.6)$$

The zero point part modifies the RPA susceptibility at $T=0$, i.e. $D_{T=0}(\underline{q}=0) = (1 - U\chi(0) - \Sigma^{I}_{T=0}(0))^{-1}$. The thermal part Σ^{I}_{T} determines the leading temperature dependence. This term is discussed in section 2c, and it is shown that

$$\Sigma^{I}_{T}\ (0) \simeq \tau^2/\alpha_0 \quad \text{for } \tau \ll \alpha_0$$

and

$$\simeq \tau \qquad \text{for } \alpha_0 \leq \tau \ll 1 .$$

Now consider a higher order diagram, e.g. Fig. 2d. Again breaking up the internal spin fluctuation energy integral into thermal and zero point parts, one gets diagrams schematically shown in Fig. 3. The Fig. 3a adds to the T=0 self energy. Fig. 3b and 3c have the same T dependence as Fig. 2g. These are 'vertex' corrections to Fig. 2a and are of O(1)[10,47] due to the intermediate coupling ($U\rho_{\varepsilon_F} \sim 1$) nature of the system. Clearly they cannot be calculated reliably. We take the point of view that these corrections can all be lumped together into vertices, i.e. Fig. 3a-3c can be redrawn as Fig. 3e-3g. Further, since these vertices again have a range ε_f in energy and k_f in

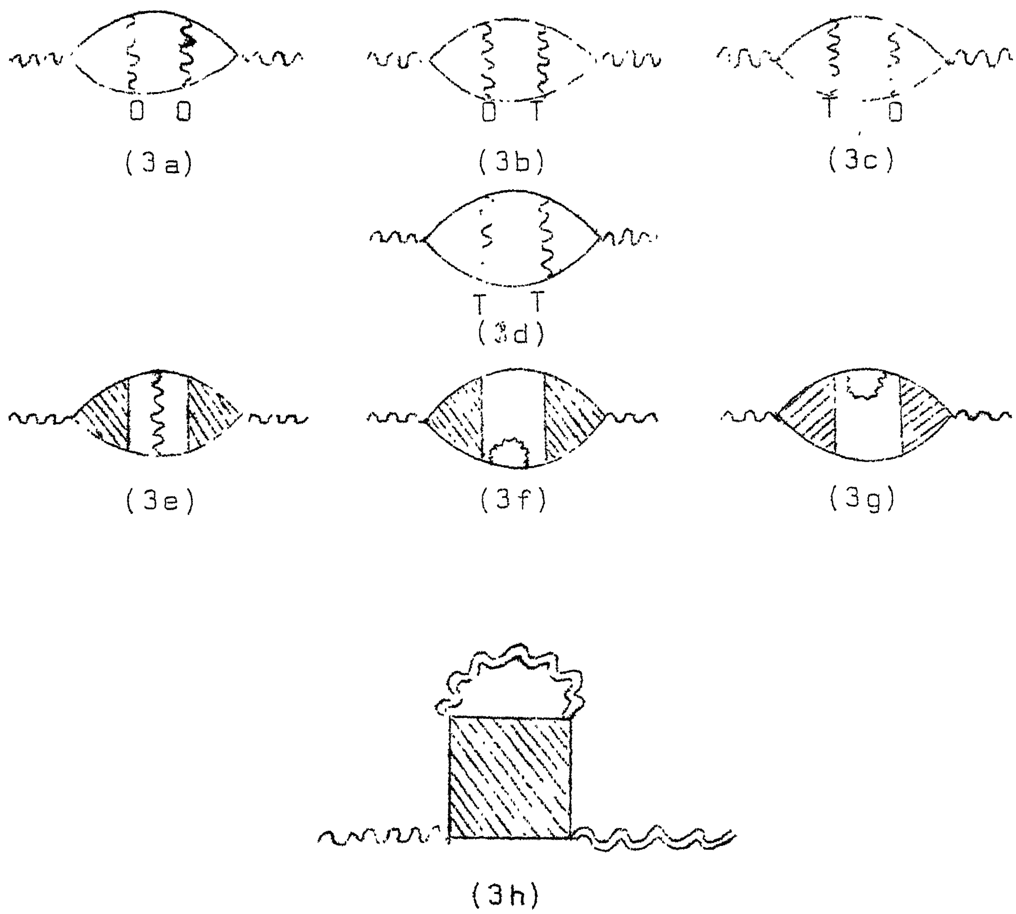


Fig. 3. Higher order diagrams and their temperature dependences.

momentum, the leading order thermal effects are given by neglecting their $\vec{q},\omega$ dependence. Thus the fully dressed thermal one spin fluctuation self energy Σ^{I} is given in Fig. 3h, where the hatched square represents a constant in which all vertex corrections have been included. This constant cannot be calculated reliably from first principles.

The last diagram, Fig. 3d, involves two thermal spin fluctuations. Because of the short range of the fermion induced coupling this will go roughly as $(\Sigma_T^I)^2$, and is thus not of the leading order in temperature. However, this conclusion is not correct if the two internal fluctuations are strongly correlated, e.g. Fig. 2e. Here, for external $\underline{q}=0$, the internal lines have four momentum $\underline{q}_1$ and $-\underline{q}_1$. The thermal part of such a diagram can be large if the coupling vertex  is sizeable. A similar analysis can be done for three internal spin fluctuation terms. We shall examine these corrections in sections 2d and 2e.

The above discussion illustrates our approach, which can be summarized as follows.

(i) Because of the intermediate coupling nature of the problem, T=0 properties cannot be calculated accurately; therefore, $\chi_{T=0}$ and the fluctuation coupling vertices cannot be accurately determined.

(ii) The temperature dependence of Σ arises from coupling to thermal spin fluctuations. The temperature dependence arising from various spin fluctuation coupling processes can be analyzed, according to the number of thermal spin fluctuations involved.

We now analyze the temperature dependence of Σ in detail, starting with one s.f. diagram and then calculating the effects of two and three internal spin fluctuations.

2c. One Spin Fluctuation

As discussed earlier this term is given by

$$\Sigma^{I}(0,0) = -\frac{\lambda}{\beta} \sum_{\underline{q}} D(\underline{q}). \tag{2c.1}$$

This leads to

$$D(q) = (1 - U\chi^{0}(\underline{q}) + \frac{\lambda}{\beta} \sum_{\underline{q}'} D(\underline{q}'))^{-1} : \tag{2c.2}$$

an equation for $D(\underline{q})$ which has to be solved self consistently for $\underline{q}=0$ to extract the temperature dependence of $\chi(T)$. In order to calculate the frequency and wave vector summation in 2c.1, an explicite dependence of D on $\vec{q}$ and ω is required. We use its functional form in RPA,

$$D^{0}(\underline{q}) = \frac{1}{1 - U\chi^{0}(\vec{q}, z_m)} \tag{2c.3}$$

$\chi^{0}(q, z_m)$ is related to the spin susceptibility of a free Fermi gas. It is given in terms of the well known Lindhard

function $F(\vec{q},\omega)$. This function has a fairly complicated dependence on its arguments. But for $q << k_f$ and $(\omega/qv_f) << 1$ we have

$$\chi^{oA}(q,\overset{\pm}{\omega}) = (\rho_{\epsilon_f})\ (1 - \delta q^2 \pm \frac{i\pi\gamma\omega}{qv_f}) \ . \tag{2c.4}$$

The small $|\vec{q}|$ and ω region is obviously the most important. In order to calculate $\chi(T)$ in various temperature regions of physical interest, we use the form (2c.4) and assume it to be valid through out. The error thus introduced is not large. With the approximation (2c.4) and following the discussion in the previous section, we can write the equation for D as follows:

$$D(\underline{q}) = \frac{1}{(\alpha(T) + \delta q^2 - \frac{i\pi\gamma\omega}{qv_f})} \tag{2c.5}$$

where

$$\alpha(T) = \alpha_o + \lambda(\frac{1}{\beta}\sum_{\underline{q}'} D(\underline{q}'))_{thermal} \tag{2c.6}$$

and $\alpha_o = (D(T=0))^{-1}$.

This α_o (and hence $\alpha(T)$) are related to Stoner enhancement factors by $\alpha^{-1}(T) = \alpha_S^{-1}(T) + 1$. $\alpha(T)$ is obtained by evaluating the integral in (2c.6) using eqn. (2c.4) with the parameters $\delta = 1/12\ k_f^2$ and $\gamma = 1/2$ (for free fermi gas). This is done below. The energy summation is easily carried out.

$$\frac{1}{\beta}\sum_{z_m} D(\vec{q},z_m) = \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\ \frac{Im\, D(\vec{q},\bar{\omega})}{e^{\beta\omega}-1}$$

$$= \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\ \frac{(\pi\gamma\omega/qv_f)(e^{\beta\omega}-1)^{-1}}{(\alpha+\delta q^2)^2 + (\frac{\pi\gamma\omega}{qv_f})^2} \tag{2c.7}$$

The integral (2c.7) can be split into two parts, a zero point part and a thermal part.

$$\int_{-\infty}^{\infty} \phi(\omega) \frac{1}{e^{\beta\omega}-1} d\omega = \int_{0}^{\infty} \phi(\omega)\, d\omega + 2\int_{0}^{\infty} \phi(\omega)\, (e^{\beta\omega}-1)^{-1}\, d\omega.$$

We have already discussed about the former one. The energy integration can be evaluated[48] for the thermal part, leading to

$$\frac{1}{\beta} \sum_{z_m} D(\vec{q}, z_m) = \frac{1}{\pi} C_q^{-1} \{\ln y - (2y)^{-1} - \psi(y)\} \qquad (2c.8)$$

where

$$C_q \equiv \frac{\gamma\pi}{q v_f},$$

$$y \equiv (\alpha(T) + \delta q^2)(2\pi k_B T\, C_q)^{-1} \qquad (2c.9)$$

and $\psi(y)$ is the digamma function. Now in order to integrate over $\vec{q}$, we need some simpler approximate form of the function,

$$\phi(y) \equiv \ln y - (2y)^{-1} - \psi(y). \qquad (2c.10)$$

Let us look at its asymptotic forms. For $y \gg 1$

$$\ln y - \frac{1}{2y} - \psi(y) = \frac{1}{12y^2} - \frac{1}{120y^4} + \frac{1}{252y^6} \qquad (2c.10a)$$

and for $y < 1$

$$\psi(y) = -\frac{1}{y} + \psi(1) + y\zeta(2) - y^2\zeta(3) + \cdots$$

$$\ln y = y-1 - \frac{1}{2}(y-1)^2 + \frac{1}{3}(y-1)^3 - \ldots$$

$$|y-1| \leq 1,\ y \neq 0$$

which imply

$$\phi(y) = y - 1 - \frac{1}{2y} + \frac{1}{y} - \psi(1) \ldots$$
$$= 1/2y \qquad y < 1 \quad . \tag{2c.10b}$$

Thus

$$\phi(y) = \frac{1}{12y^2} \qquad y \gg 1$$
$$= \frac{1}{2y} \qquad y < 1 \quad .$$

A good and simple interpolation formula applicable over the temperature range of interest is

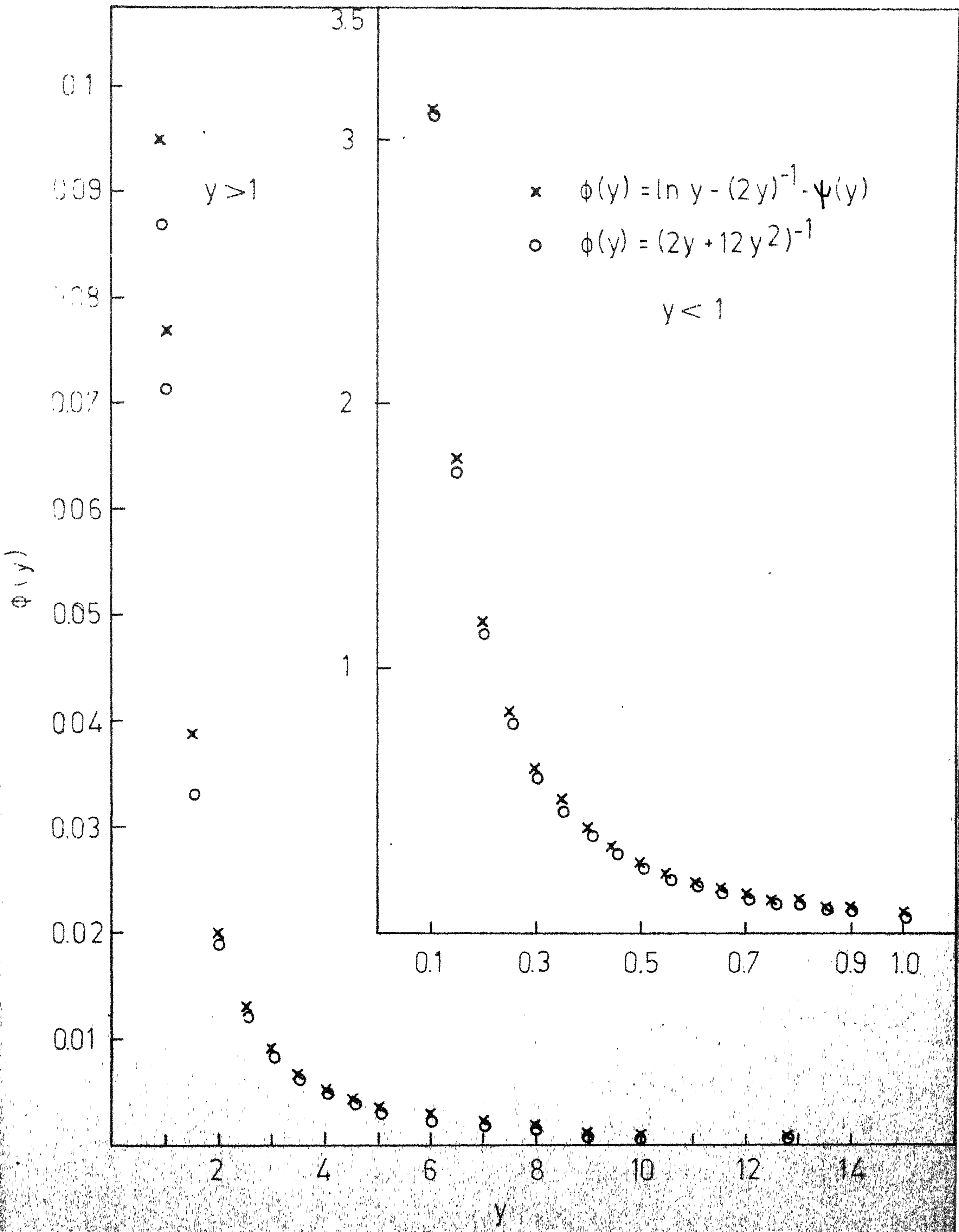
$$\ln y - \frac{1}{2y} - \psi(y) = \frac{1}{2y + 12y^2} \quad . \tag{2c.11}$$

A comparison between left and right hand side is shown in Fig. 4. Using this, the momentum integration can be carried out. Before performing explicit numerical calculation, let us first investigate different temperature regions of physical interest. From our experience with the paramagnon theory and the experimental results, we see that there are two such regions.

(i) <u>The Paramagnon regime</u> : This is defined by the inequality $y \gg 1$, i.e.

$$(\alpha + \delta q^2)\ qv_f/2\pi^2 \gamma k_B T \gg 1$$

which implies $\tau/\alpha_0 \ll 1$. Consider the first term in the expansion of $\phi(y)$ in eqn. (2c.10a), and substitute in the integral



3.5
0.1
3
0.09
y > 1
ϕ(y) = ln y - (2y)^-1 - ψ(y)
ϕ(y) = (2y + 12y²)^-1
0.08
y < 1
0.07
2
0.06
ϕ(y)
0.05
1
0.04
0.03
0.02
0.1
0.3
0.5
0.7
0.9
1.0
0.01
2
4
6
8
10
12
14
y

Fig. 4.

$$\sum_{\vec{q}} D(\vec{q}) = \frac{1}{\pi} \sum_{\vec{q}} C_q^{-1} \frac{1}{12y^2} . \qquad (2c.12)$$

This integral can be calculated. It is cut off independent and the result is

$$\sum_{\vec{q}} D(\vec{q}) = \frac{\Omega}{12v_f} (\frac{\gamma}{\delta}) \frac{(k_B T)^2}{\alpha_o} \qquad (2c.13)$$

for $\tau << \alpha_o$. This is the T dependence we get in the paramagnon theory. Note that the calculation is not performed self consistently. The leading correction to above result can be calculated by taking the next term in the expansion.

$$\Delta(\sum_{\vec{q}} D(\vec{q}))$$

$$= \frac{1}{\pi} \sum_{\vec{q}} C_q^{-1} (- \frac{1}{120}) \frac{1}{y^4} \qquad (2c.14)$$

The integral turns out to be like $\int dq\, q^{-1}(\alpha + \delta q^2)^{-4}$. There seems to be a logarithmic divergence for small q, but this is spurious since we have a lower cut off in this limit, i.e. $q > q_c = (2\pi^2\gamma/v_f)\ (k_B T/\alpha_o)$. Considering this we obtain to the lowest order in τ.

$$\Delta(\lambda \sum_{\vec{q}} D(\vec{q})) = \frac{\tau^4}{\alpha_o^4} \ln \frac{\tau^2}{\alpha_o^3} , \qquad (2c.15)$$

which means that the result 2c.13 is correct if $\tau^2/\alpha^3 \ln \tau^2/\alpha_o^3 << 1$.

Thus the leading correction to the paramagnon result is $\tau^4/\alpha_o^4 \ln \tau^2/\alpha^3$ and the approximation converges fast if $\tau^2/\alpha^3 \ln \tau^2/\alpha^3 << 1$.

(ii) Classical Curie like regime : Now we investigate the other limit: $y < 1$. This corresponds to $(\delta q^3 v_f / 2\ 2\pi\gamma k_B T) \ll 1$. The fluctuations are cut off at a momentum $\tilde{q}_c = (\frac{q_c}{k_f}) = \tau^{1/3}$. There is no restriction on temperature, except that the system is degenerate, i.e. $\tau \ll 1$. Here

$$\sum_{\vec{q}} D(\vec{q}) = \frac{1}{\pi} \sum_{\vec{q}} C_q^{-1} \frac{1}{2y} \tag{2c.16}$$

$$= \frac{1}{\pi} \frac{\Omega}{2\pi} (k_B T) \int_0^{q_c} d_q \frac{q^2}{(\alpha + \delta q^2)}$$

$$= \frac{1}{2\pi^2} \left(\frac{k_B T}{\delta}\right) \{ q_c - \sqrt{\frac{\alpha}{\delta}} \tan^{-1} q_c \sqrt{\frac{\delta}{\alpha}} \} \tag{2c.17}$$

Thus the amplitude of thermal spin fluctuations is proportional to $(k_B T \rho_{\varepsilon_F}) \quad (T\rho_{\varepsilon_F})^{1/3}$. This is the same term obtained by many authors[14,15,18,20] in their analysis of itinerant ferromagnets above T_c. The term is qualitatively understood as follows. $(k_B T \rho_{\varepsilon_F})$ is the relative volume in energy space of fluctuations with energy less than $k_B T$, this cutoff arising from the thermal occupation factor $(e^{\beta\omega} - 1)^{-1}$. The volume in q space of this fluctuations contributes a further factor $(k_B T \rho_{\varepsilon_F})^{1/3}$. Because of the size of the coefficient ($\delta(\simeq .08)$ small) this term varies almost linearly with temperature. There is no thermal contribution coming from elsewhere, and for α_0 very small $\alpha(\tau)$ varies as τ. This is the desired Curie behaviour for the susceptibility. Notice that even though

the system is highly degenerate ($\tau << 1$), because of the spin fluctuations and their interaction a Curie law behaviour is obtained and the system behaves as a collection of independent classical spins. Some of the consequences of this result will be discussed in Chapter IV.

2d. Two Spin Fluctuations

It has been suggested by Ramakrishnan[18] that the contribution of two internal spin fluctuation diagrams to $\alpha(T)$ is negligibly small. This follows from the fact that in the classical limit (where only $D(\vec{q}, z_m=0)$ is considered while performing the energy sum), for $|\vec{q}| \to 0$, the contribution vanishes identically due to time reversal invariance. This is true only in the classical limit but not otherwise. Beal-Monod et al. have considered this term (they do not mention this explicitly) and obtain a contribution τ^2/α_0, same as obtained from one spin fluctuation term. We also consider this term. Though in the classical limit this is zero but it is nonvanishing in general. Following the discussion in section 2b, we consider diagrams with a momentum correlation between the internal fluctuation lines only. These diagrams are represented by Fig. 2e. There are four such diagrams, each containingone transverse and one longitudinal fluctuation line. Adding all these diagrams with proper weight factors and noting that

there is no difference in up and down spin in the paramagnetic phase, a considerable amount of simplification results and we get,

$$\Sigma^{II}(0) = \lambda_2 \frac{1}{\beta} \sum_{\underline{q}} D_{\underline{q}} D_{-\underline{q}} \phi(\underline{q}) \qquad (2d.1)$$

where

$$\phi(\underline{q}) = \{ \frac{U^2}{\beta} \sum_{\underline{k}} G_k^2 (G_{k-q} - G_{k+q}) \}^2$$

$$= 2\{ (\frac{\partial \chi^{0+-}}{\partial B})_{B=0} U^2 \}^2 \qquad (2d.2)$$

$$\lambda_2 = \frac{1}{3U}$$

The expression in the bracket { } has been calculated by Beal-Monod et al.

$$(\frac{\partial \chi^{0+-}}{\partial B})_{B=0} = 2\rho_{\varepsilon_F} \frac{\omega}{q^2 v_f^2} (1 + 0((\frac{\omega}{qv_f})^2)) + \frac{\omega}{qv_f} 0(\frac{q}{k_f})$$

$$(2d.3)$$

After substituting expressions (2d.2) and (2d.3) in (2d.1) and carrying out the energy integration, the thermal contribution to $\Sigma^{II}(0)$ is obtained as

$$\Sigma^{II}(0)|_{Thermal} = \lambda_2 \cdot \sum_q \int_0^\infty \frac{d\omega}{e^{\beta\omega} - 1} \frac{2}{\pi} Im\{D_{\underline{q}} D_{-\underline{q}}\} Re\ \phi(\vec{q}, \omega) \qquad (2d.4)$$

$$= 16\lambda_2 \rho_{\varepsilon_F}^2 \cdot \sum_q \int_0^\infty \frac{d\omega}{e^{\beta\omega} - 1} \frac{2}{\pi} \frac{2(\alpha + \delta q^2) \frac{\pi\gamma\omega}{qv_f} \cdot \frac{\omega^2 U^4}{q^4 v_f^4}}{\{(\alpha + q^2)^2 + \frac{\pi^2\gamma^2\omega^2}{q^2 v_f^2}\}^2}$$

$$= \lambda_2 \cdot 16U^2 \rho_{\varepsilon_F}^2 \{ \frac{2U^2\Omega}{\pi^4\gamma^2 v_f^2} \} k_B T \int dq\ y \int \frac{2dt}{(e^{2\pi t} - 1)}$$

$$\times \frac{t^3}{\{y^2 + t^2\}^2} \qquad (2d.5)$$

Here $t = (\beta\omega/2\pi)$ and $y = \frac{(\alpha - \delta q^2)}{2\pi^2} \frac{qv_f}{k_B T}$ as before. The integration in (2d.5) is rather complicated, but can be transformed to the integral appearing in equation (2c.7). The result is

$$\Sigma^{II}(0)|_{\text{Thermal}} = \bar{\lambda}_2 \frac{k_B T}{2} \int dq \frac{\partial}{\partial y} \{y^2 (\ln y - (2y)^{-1} - \psi(y)\} \qquad (2d.6)$$

$$\bar{\lambda}_2 = \lambda_2 \cdot 16U^2 \rho_{\varepsilon_F} \{\frac{2U^2 \Omega}{\pi^4 \gamma^2 v_f^2}\} .$$

This integral can be estimated in various temperature regimes. In the extreme paramagnon limit $\tau/\alpha << \alpha^{1/2}$ it gives a τ^2/α contribution, the next term is smaller by τ^2/α^3. In the Curie regime a $\tau^{4/3}$ term is obtained, as expected.

To summarize we emphasize that the contribution from the spin fluctuation correlation (drag) term is important and is of the same order as mean fluctuation field term (one s.f. term calculated self consistently).

2e. Three Spin Fluctuations

The results obtained in the previous two sections are useful if the fluctuation expansion is convergent, i.e. higher order corrections are small. To check this we estimate the leading contribution from the third order thermal corrections to the self energy. As in the previous

section we consider only those diagrams which have three correlated thermal fluctuations. All other diagrams can either be absorbed in one or two spin fluctuation vertices or they contribute to the order $(\Sigma^{I}(T))^{3}$ or $(\Sigma^{I}(T))^{2}$, which is small. The resulting self energy diagram is shown in Fig. (2f). The internal fluctuation lines can be one transverse and two longitudinal or all three transverse. Now there are various ways of joining fluctuation lines and the four fermion vertices, e.g. Fig. (5a,b&c). Taking into account all the combinatorial factors, we can write down the expression for the self energy as

$$\Sigma^{III}(\underline{q}) = \lambda_3 \cdot \frac{1}{\beta^2} \sum_{\underline{q}_1 \underline{q}_2} D(\underline{q}_1)\ D(\underline{q}_2)\ D(\underline{q}-\underline{q}_1-\underline{q}_2) \tag{2e.1}$$

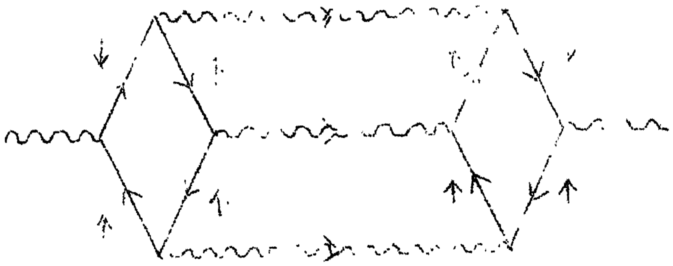
with

$$\lambda_3 = \frac{8}{15U^2} \left\{ \frac{U^3}{\beta} \sum_{\underline{k}} G^4_{\underline{k}} \right\}^2$$

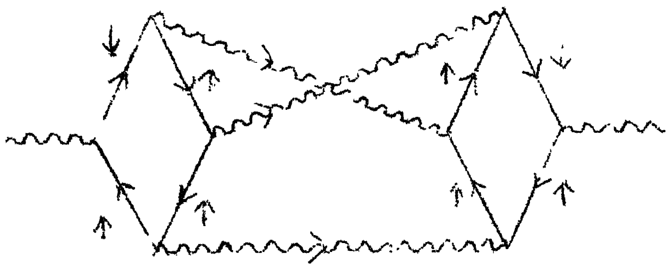
$$= \frac{8}{15U^2} \left\{ U^3 \frac{\rho''_{\varepsilon_F}}{6} \right\}^2 .$$

Here we have assumed the four fluctuation vertex to be of zero range and energy independent. This is done by considering only $\underline{q}=0$ term in the momentum expansion of the product of the four Fermion propagators constituting the vertex. Writing equation (2e.1) in terms of spectral functions,

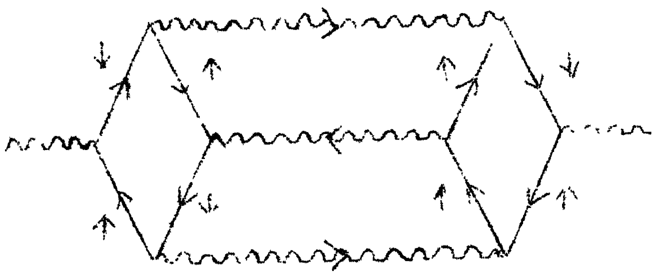
$$\Sigma^{III}(\underline{q}) = \lambda_3 \sum_{\vec{q}_1 \vec{q}_2} \int \prod_i d\omega_i \ \frac{\rho_{q_1}(\omega_1)}{\omega_1 - z_1} \ \frac{\rho_{q_2}(\omega_2)}{\omega_2 - z_2} \ \frac{\rho_{q-q_1-q_2}(\omega_3)}{\omega_3 - z + z_1 + z_2} . \tag{2e.2}$$



(5a)



(5b)



(5c)

Fig. 5. Some three correlated spin fluctuation diagrams.

After performing the frequency summation (over z_1 and z_2) and some algebra, we see that pure thermal contribution to $\Sigma^{III}(0)$ is given by

$$\Sigma^{III}(0) = -2\lambda_3 \sum_{\vec{q}_1,\vec{q}_2} \int_0^\infty \prod_i d\omega_i \; \frac{\rho_1(\omega_1)\ \rho_2(\omega_2)\ \rho_3(\omega_3)}{\omega_1 + \omega_2 + \omega_3}$$

$$\times\ g(\omega_1)\ g\ (\omega_2)\ g(\omega_3) \qquad (2e.3)$$

Now one has three possible temperature contributions from the Bose functions $g(\omega)$, viz. one thermal, two zero point; two thermal, one zero point and all three thermal contributions. The first and second terms will only modify the coefficients of the results obtained in the previous sections. The leading characteristic thermal correction comes only from the third one. In the classical (thermal) approximation with an appropriate cut off ($\sim k_BT$) i.e. with

$$\omega_1 + \omega_2 + \omega_3 \sim k_BT,$$

$$\int_0^\infty \frac{F(\omega)d\omega}{e^{\beta\omega}-1} \sim \int_0^{\eta k_BT} \frac{F(\omega)d\omega}{\beta\omega}$$

and $\eta \sim 1$; the energy integral can be estimated to give

$$\Sigma^{III}(0) = -2\lambda_3(k_BT)^2 \sum_{\vec{q}_1,\vec{q}_2} \int_0^{\eta k_BT} \prod_i d\omega_i \; \frac{\rho_1(\omega_1)\rho_2(\omega_2)\rho_3(\omega_3)}{\omega_1\ \omega_2\ \omega_3}$$

$$(2e.4)$$

Using

$$\rho(\vec{q},\omega) = \frac{1}{\pi}\ \mathrm{Im}\ D(\vec{q},\omega^-) = \frac{1}{\pi}\ \frac{(\pi\gamma\omega/qv_f)}{(\alpha+\delta q^2)^2 + (\frac{\pi\gamma\omega}{qv_f})^2} \qquad (2e.5)$$

the energy integration can be performed and the result is

$$\Sigma^{III}(0) = -2\lambda_3 \ (k_B T)^2 \ (\tfrac{1}{\pi})^3 \sum_{\vec{q}_1, \vec{q}_2} \frac{1}{\alpha + \delta q_1^2} \ \frac{1}{\alpha + \delta q_2^2} \ \frac{1}{\alpha + \delta |\vec{q}_1 + \vec{q}_2|^2}$$

$$\times \prod_i \tan^{-1} \theta_i \qquad (2e.6)$$

with $\theta_i = \dfrac{\eta \, k_B T \ \gamma\pi}{(\alpha + \delta q_i^2) \ q_i v_f}$.

The temperature dependence of Σ^{III} comes from a factor $(k_B T)^2$ outside the integral and the angles $\tan^{-1} \theta_i$. Its behaviour can now be studied in two different temperature regimes.

(i) For very low temperatures, $\tau << \alpha$

$$\Sigma^{III}(0) = -2\lambda_3 \ (k_B T)^2 \ (\tfrac{1}{\pi})^3 \ \frac{\Omega^2}{(2\pi)^6} \ 8\pi^2 .$$

$$\int_0^{q_c} \frac{q_1^2 dq_1}{(\alpha + \delta q_1^2)^2} \int_0^{q_c} \frac{q_2^2 \ dq_2}{(\alpha + \delta q_2^2)^2} \int_{-1}^{1} dt \ \frac{(\eta \, k_B T \ \gamma \, \pi)^2}{v_f^2 \ q_1 \ q_2}$$

$$\frac{1}{\alpha + \delta |\vec{q}_1 + \vec{q}_2|^2} \ . \qquad (2e.7)$$

where we have made the following approximations:

(a) $\tan^{-1} \theta_1 = \theta_1$ for two of the angles, since $\theta_1 > \tan^{-1} \theta_1$. This can at the most lead to an overestimate.

(b) $\tan^{-1} \theta_3 = 1$ for one of the angles. Now $(\tan^{-1} \theta_3)_{max} = \pi/2 = 1.57$. Generally, for small T, $\theta_3 \propto \tau << \pi$, this is also

an overestimate. This simplifies the integration considerably. Now the integral over t becomes

$$\int_{-1}^{1} dt\{\alpha + \delta(q_1^2 + q_2^2 + 2q_1q_2t)\}^{-1} = \frac{1}{2\delta q_1 q_2} \ln \frac{\alpha+\delta(q_1+q_2)^2}{\alpha+\delta(q_1-q_2)^2}$$

which is non singular as $\alpha \to 0$, and always positive. The singularity at $q_1 = q_2$ is mild and integrable. Therefore $\ln \left(\frac{q_1 + q_2}{q_1 - q_2}\right)^2 \sim 1$. Then

$$\Sigma^{III}(0) = A\ I^2 \text{ where } I = \int_0^\infty \frac{dq}{(\alpha + \delta q^2)^2} = \frac{\pi}{4\delta^{1/2}\ \alpha^{3/2}}$$

and $A = \text{constt.}\ \lambda_3\ \tau^4$.

This gives

$$\Sigma^{III}(0) = \text{Constt.}\ \tau^4/\alpha^3 ,$$

which is small by a factor of $(\tau/\alpha)^2$ compared to one spin fluctuation term in this regime.

(ii) In the classical Curie regime ($\alpha_0 \leq \tau << 1$) since the temperature is higher $\tan^{-1}\theta$ factors can be approximated as 1. The remaining integral becomes

$$\Sigma^{III}(0) = -2\lambda_3\ (k_B T)^2\ \left(\frac{\Omega}{8\pi^3}\right)^2$$

$$\int d^3q_1 d^3q_2\ \frac{1}{\alpha + \delta q_1^2}\ \frac{1}{\alpha + \delta q_2^2}\ \frac{1}{\alpha + \delta|\vec{q}_1 + \vec{q}_2|^2} \tag{2e.8}$$

which can be evaluated.[49] The final result is

$$\Sigma^{III}(0) = B\ T^2\ \ln\left(\frac{1}{3\alpha}\right), \tag{2e.9}$$

in contrast to the linear T dependence in one spin fluctuation approximation in this temperature range.

Thus we see that spin fluctuation correlation correction term is smaller, by a factor $(\tau/\alpha)^2$ in the paramagnon regime and by τ in the Curie regime than the mean fluctuation field term. Therefore, as far as the temperature dependence is concerned, the higher order spin fluctuation effects are quite small.

3. Comparison with Experiments on Liq He^3

There are many metals and alloys which are nearly ferromagnetic and our results can be compared with X(T) observed in them. Since Liq He^3 is a 'clean' case, i.e. there are no band structure complications, we study it in detail. In their paper II,[25] J. R. Thompson et al. have discussed X(T)/C from 0.03°K to 2.2°K and for ten molar volumes ranging from 26.5 cm^3/mole to 35.5 cm^3/mole. The two extreme cases i.e. highest density (26.5 cm^3/mole) and the lowest (35.5 cm^3/mole) are considered here. These correspond to free fermi gas degeneracy temperatures 6.18°K and 5.08°K respectively. The Stoner enhancement factor $\alpha^S(T)$, is a quantity of interest. We transform both the observed and calculated numbers to it:

$$\alpha^{S}(T)^{-1} = \chi(T)/\chi_P$$

$$= \alpha^{-1}(T) - 1$$

$$= \frac{2}{3}\ (\chi/L)\ T_F^{o}\ .$$

The contribution due to one spin fluctuation is given by equations (2c.5) and (2c.6) which, for computational purposes, can be written as

$$\alpha_1(T) = \alpha(0) + \Lambda_1 \int_0^{q_c} dq \frac{q^3}{2y + 12y^2} \tag{3.1}$$

where the 'bare'

$$\Lambda_1 = \frac{5}{6\pi^2\ \gamma} \left(\frac{2}{3}\right)^2 (U\rho_{\varepsilon_F})^2 .$$

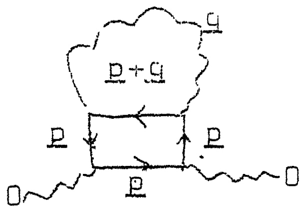
Other functions are defined as

$$y = \frac{(\alpha(T) + \delta q^2)\ q}{\pi^2\ \gamma\ \tau}\ ,\quad \delta = 1/12,\ \gamma = 1/2,\ \tau = T/T_F^{o},\ \text{and}$$

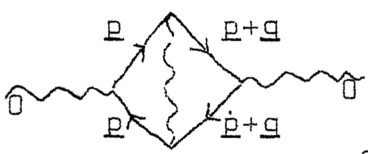
$q = q/k_f^{o}$.

In writing (3.1) we have made several approximations. Firstly, we have assumed that $\chi^{o}(\vec{q})$ can be written as $\chi^{o}(0)$ $(1 - \delta q^2)$ for values of q of interest to us. For $q = 2k_f$ this leads to a value $\chi^{o}(0) \simeq 0.33$ whereas the actual value is $\chi^{o}(0) \simeq 0.5$. For smaller q, the discrepancy is much smaller. (We can use full Lindhard function instead of the approximate form, but this does not lead to significantly different numbers.) Further, we have approximated

the fact that the quartic s.f. coupling goes to zero naturally for large q by a very simple cut off $\theta(q-q_c)$. Now the spin fluctuation vertex form factor can, in principle, be calculated in the lowest order, e.g., one can calculate for a diagram,



the vertex to be $\sim \sum_{\underline{p}} [G_{\underline{p}}^{3}(G_{\underline{p}+\underline{q}} + G_{\underline{p}-\underline{q}})]$. This decreases rapidly for large q. The other spin fluctuation coupling diagram



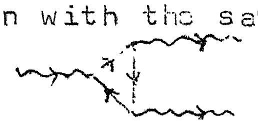
has its vertex going as $\sum_{\underline{p}} (G_{\underline{p}}^{2} G_{\underline{p}+\underline{q}}^{2})$. This clearly has a different large q dependence. Further, vertex corrections are of relative order unity and will alter the q dependence. For small q ($\lesssim k_f$) and rigorously in the zero q limit, these two vertex terms coincide. Taking all this into consideration, for simplicity, therefore we adopt a form which treats all quartic vertex terms identically, and simulates the large q decrease by a single sharp cut-off. The magnitude Λ_1 of the vertex is treated as an adjustable parameter. This is reasonable because the four s.f. vertex cannot be calculated accurately. Corrections are of order unity. For a given q_c, we fix Λ_1 by fitting to the low temperature data ($\tau \leq \alpha_0$) where $\chi^{-1} = \chi^{-1}(0) + \Lambda\tau^2$.

If fluctuations in the same q range determine $\chi^{\cdot}$ at all temperatures, and our simple representation of the vertex is fairly realistic, we expect a good fit at all temperatures. $\alpha(0)$ is fixed by $\chi(T=0)$. Non-selfconsistent results are obtained by substituting α_o for $\alpha(T)$ in y at all temperatures and obtaining $\alpha(T)$ from (3.1). Otherwise $\alpha(T)$ is calculated self-consistently.

The two s.f. contribution (Eqn. 2d.6) can be written as

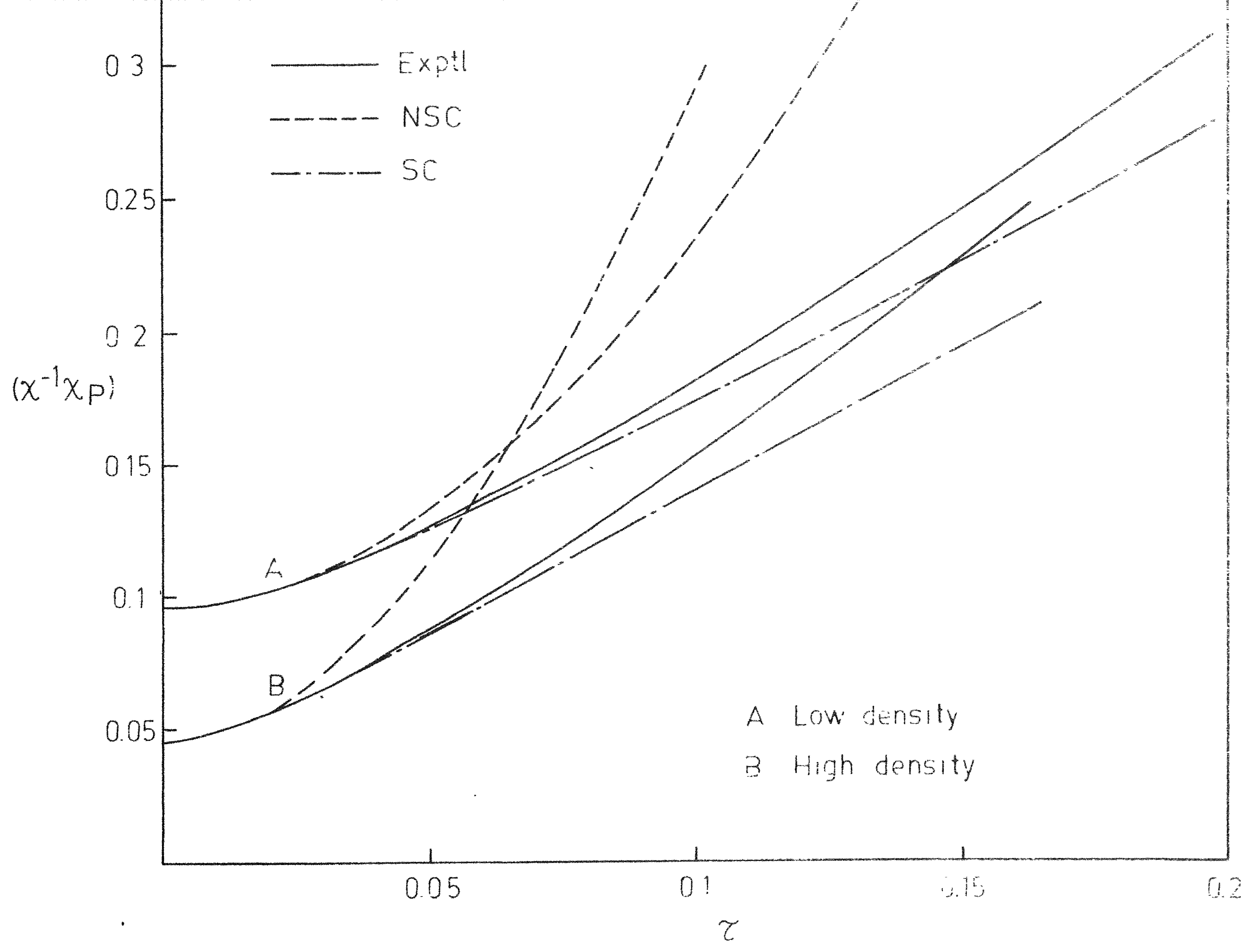
$$\alpha(T) = \alpha_1(T) - \Lambda_2 \, \tau \int_0^{q_c} \frac{dq}{(1 + 6y)^2} \qquad (3.2)$$

with $\Lambda_2 = \frac{8}{3\pi^2 \gamma^2} \left(\frac{2}{3}\right)^3 (U\rho_{\varepsilon_F})^3$.

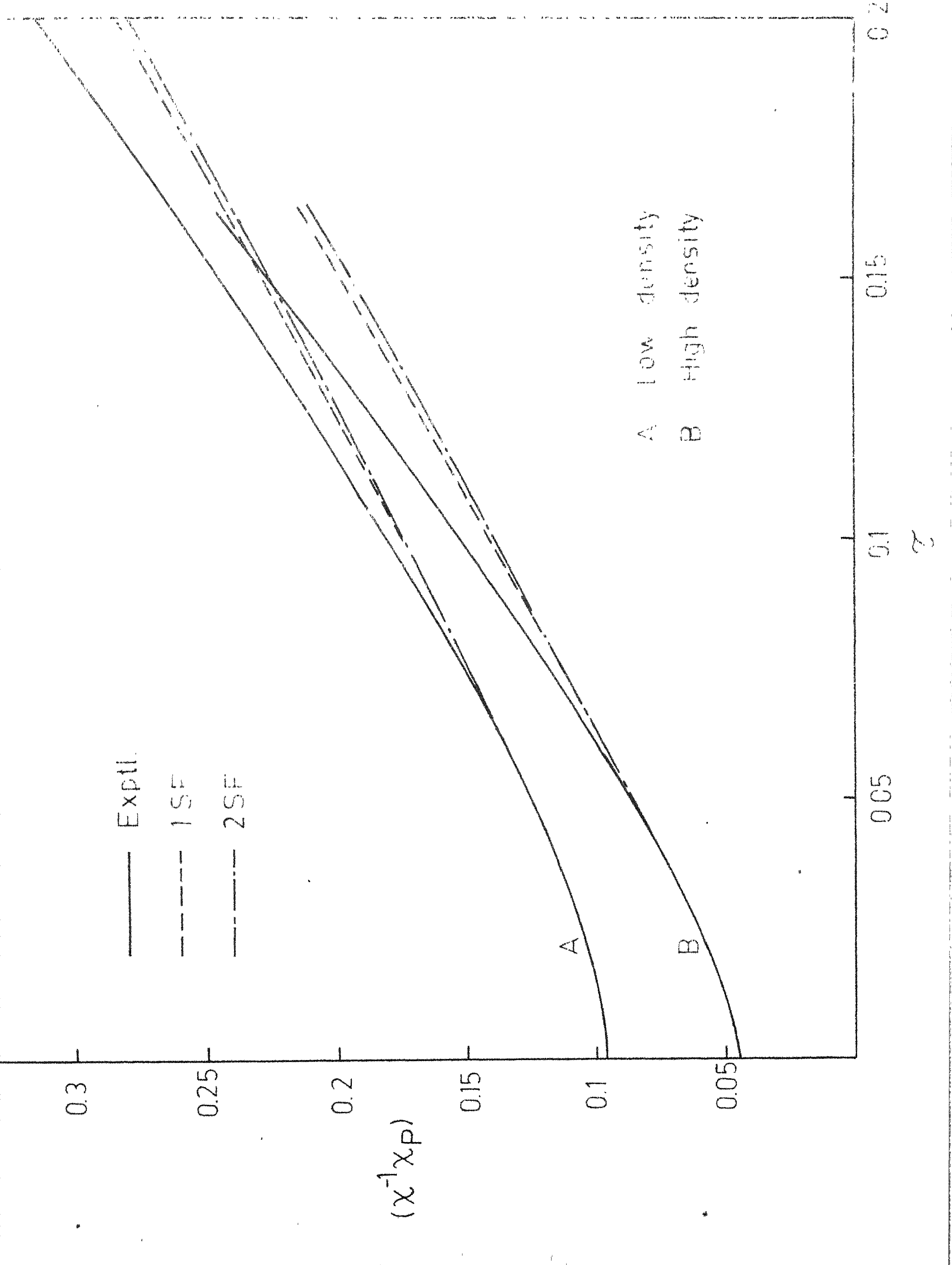
Now even with the same simple cutoff model for the two s.f. vertex , there is one more parameter, i.e. the size Λ_2 of the vertex. We fix it as follows. Calculations show that the two s.f. term contributes about 15% of the one s.f. term and has the same temperature dependence. So for simplicity, we choose for Λ_2 the bare value, keeping only Λ_1 as a free parameter. Again self-consistent and non-selfconsistent calculations for $\alpha(T)$ have been performed.

The parameters α_o and Λ_1 are given in Table I. The results are shown in Figures 6, 7 and 8. It is clear

that qualitatively there is no difference between one and two s.f. contributions if the calculations are performed self consistently. Both of these agree with experiment over a wide temperature range ($\tau \leq 0.2$). The agreement becomes progressively poorer. The non-selfconsistent calculation gives good results in the very low temperature region only. This is the reason why the results of Beal-Monod et al. do not hold beyond $\tau = 0.2\ \alpha_o$. The non-self consistent formula drastically overestimates the fluctuation effect for $\tau > 0.2\ \alpha_o$. In formal terms the effect of self consistency is seen as follows. The low temperature deviation of $\alpha(T)$ from $\alpha(0)$ is $A\tau^2/\alpha$. That is, $\alpha(\tau) - \alpha(0) = \dfrac{A\tau^2}{\alpha(0) + A\tau^2/\alpha}$. Clearly for $\alpha(0) >> \dfrac{A\tau^2}{\alpha}$, there is no difference between the self consistent and the non-self consistent values. But beyond this narrow range, the difference begins to increase. It is also easy to see that the leading self consistency correction term $- A^2\tau^4/\alpha^3(0)$ has the same α^{-1} dependence as the three spin fluctuation term which is also of the form τ^4/α^3. Thus, self consistency effects are not very important for $\tau << \alpha_o$. However, in the classical regime where the corresponding quantities are τ^2/α and $\tau^2 \ln 1/\alpha$ respectively, the difference is very large. Thus, it is important to keep the calculation self consistent.



Exptl
NSC
SC
A
B
A Low density
B High density
$(\chi^{-1}\chi_P)$
0.3
0.25
0.2
0.15
0.1
0.05
0.05
0.1
0.15
0.2
τ



0.3
0.25
0.2
0.15
0.1
0.05
$(\chi^{-1}\chi_P)$
0.05
0.1
0.15
0.2
τ
A
B
Exptl.
1SF
2SF
A Low density
B High density

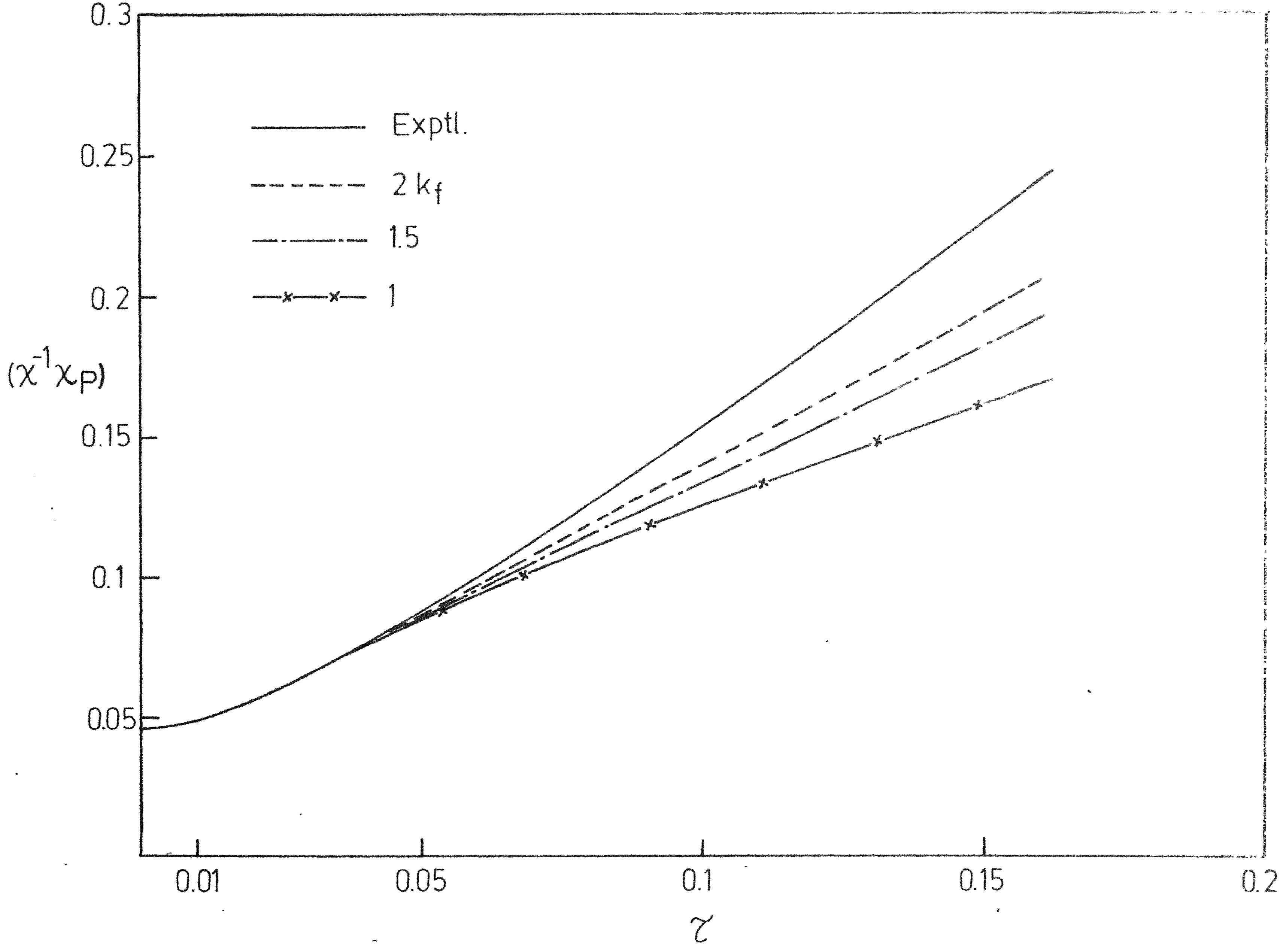

0.3
0.25
0.2
0.15
0.1
0.05
$(\chi^{-1}\chi_P)$
Exptl.
$2\,k_f$
1.5
1
0.01
0.05
0.1
0.15
0.2
τ

Fig. 8.

We notice also that Λ_1 changes only weakly as we go from the $\alpha_o = .1$ to $\alpha_o = .05$ case. This is understandable since Λ_1 depends on T_F or density which does not change much. The value of the coupling Λ_1 depends strongly on cut off being nearly inversely proportional to it. This is not surprising since the fluctuation excitation energy goes up only slowly with q (δ small). Thus a considerable part of q space is involved, and cutting off a sizeable segment of it needs to be compensated by increase in Λ_1. At low temperatures ($\tau << \alpha_o$) where cut off dependence of $\alpha(\tau)$ be analytically obtained, the results broadly verify our numerical result.

Now we estimate the higher order corrections due to Σ^{III}. For $\alpha_o \leq \tau << 1$ where the departure becomes sizeable, Eqn. (2e.8) and (2e.9) give

$$\Sigma^{III} = -\lambda_3 \; (k_B T)^2 \; \frac{\Omega^2}{(2\pi)^6} \; (2k_f)^6 \; \frac{4\pi^4}{\delta\; 3} \; \ln \; (1/3\alpha_o^s) \qquad (3.3)$$

with $\lambda_3 = \frac{8}{15U^2} \left(\frac{U^3 \rho_{\varepsilon_F}}{24\varepsilon_F^2}\right)^2$ and $\bar{\delta} = 1/3$, the correction term can be written as

$$\Sigma_T^{III} = -\frac{8}{5} \pi^2 \; (U\rho_{\varepsilon_F})^4 \; \left(\frac{2}{3}\right)^4 \; \tau^2 \; \ln \; (1/3 \; \alpha^s).$$

This gives a positive contribution to $\alpha(T)$ and moreover $\Delta\alpha(T)$ is .02 and .01 at $\tau = .1$, and .05 and .026 at $\tau = .15$ for high density and low density respectively. This is of the same order as $\Delta(\alpha_{EXPT} - \alpha_{TWO\ S.F.})$.

Table I

Low density

$V_m = 35.5\ cm^2/mole$

$T_F^o = 5.08°K$

q_c		1	1.5	2
1 S.F.	α_o	.0870	.0874	.0876
	Λ_1	.3356	.2018	.1592
2 S.F.	α_o	.0870	.0874	.0876
	Λ_1	.3755	.2266	.1790

High density

$V_m = 26.5\ cm^3/mole$

$T_F^o = 6.18°K$

q_c		1	1.5	2
1 S.F.	α_o	.0418	.0426	.0430
	Λ_1	.3264	.2120	.1592
2 S.F.	α_o	.0418	.0426	.0430
	Λ_1	.3622	.2360	.1956

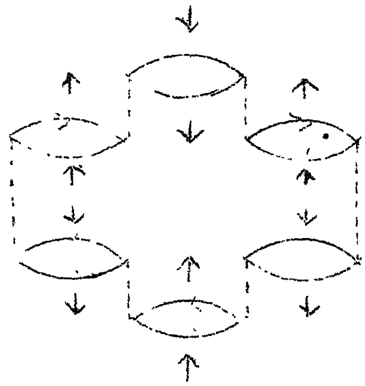
4. Comparison with Earlier Work

There have been several attempts to study $\chi(T)$ of highly paramagnetic metals, alloys and Liq He^3, but the results disagree in many respects. For low temperatures $\tau << \alpha_o$, Beal-Monod et al.,[13] Kawabata[21] and we find a doubly enhanced T^2 variation due to a contribution from spin fluctuations (Eqn. 4.1). These results disagree with the singly enhanced T^2 term of Stoner's theory. Misawa[40] and Barnea[39] obtain a completely different temperature dependence. On the basis of phenomenological Landau theory Misawa gets a T^2 ln T variation with a singly enhanced coefficient, while Barnea in a microscopic Landau theory gets a triply enhanced coefficient (Eqn. 4.2).

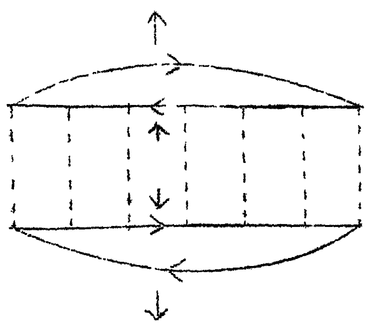
$$\chi(T) = \chi(0) [1 - \alpha' (\frac{T}{\alpha_o T_F})^2] \qquad (4.1)$$

$$\chi(T) = \chi(0) [1 - \alpha_M \frac{T^2}{T_F^2 \alpha_o^3} \ln (\frac{T}{\alpha_o T_F})] \qquad (4.2)$$

The expression (4.2) exhibits a peak in $\chi(T)$ at a temperature $\alpha_o T_F/\sqrt{e}$, while expression (4.1) does not. A peak in $\chi(T)$ is observed in many systems, e.g. Pd, α-Mn, U_2C_3, N_pCo_2, YCo_2, etc. This $\chi(T)$ maximum is 'explained' as being due to a nearly ferromagnetic fermi system obeying the above T^2 ln T 'law'. There are many systems, e.g., Ni_3Ga, $HfZn_2$, Liq He^3, Ni-Rh etc. which can equally well be described as nearly ferromagnetic fermi liquids and which do not show any peak.



(9a)



(9b)

Fig. 9. Ring and ladder diagrams entering in ΔF.

An expression for ΔF can be read out from the usual rules and the result is

$$(\frac{N}{V})\ \Delta F_{ring} = \frac{1}{2} \sum_{\underline{q}} \{\ln\ (1-U^2\ \chi^{o+}_{\underline{q}}\ \chi^{o-}_{\underline{q}}) + U^2 \chi^{o+}_{\underline{q}} \chi^{o-}_{\underline{q}}\}$$

$$(\frac{N}{V})\ \Delta F_{ladder} = \sum_{\underline{q}} \{\ln\ (1-U\ \chi^{o+-}_{\underline{q}}) + U\ \chi^{o+-}_{\underline{q}}\}\ . \qquad (4a.2)$$

An expression for $\Delta\chi$ can be written down in terms of the free energy ΔF, as

$$\Delta\chi = -(\frac{\chi(T)}{\chi(0)} - 1)$$

$$= \frac{2}{3}\ \frac{T_F}{\alpha_o}\ \frac{\partial^2\ \Delta F}{\partial B^2}\bigg|_{B=0}\ . \qquad (4a.3)$$

If we differentiate ΔF twice with respect to B (diagrammatically), we get the following set of diagrams (Fig. 10). Clearly contributions from one and two, longitudinal and transverse internal spin fluctuations, have been considered. Ignoring the temperature correction to $\mu_{T=0}$ at low temperatures† and considering terms divergent for $\alpha \to 0$, one gets

$$(\frac{N}{V})\ (\frac{\partial^2}{\partial B^2}\ \Delta F_{ring})_{B=0} = \frac{T^2}{2\alpha_o} + O\ (\ T^4\ \ln\ T)$$

and

$$(\frac{N}{V})\ (\frac{\partial^2}{\partial B^2}\ \Delta F_{ladder})_{B=0}$$

$$= \frac{T^2}{\alpha_o}\ [\,(\frac{1}{6} - \frac{4}{3\pi^2}) + \frac{8}{3\pi^2}\ (\frac{4}{\pi^2} - 1)\ \alpha_o\ \ln\ \alpha_o\,]$$

$$+\ O\ (T^4\ \ln\ T) \qquad (4a.4)$$

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†As shown by Beal-Monod et al.[13] ΔF is to be calculated with the free energy function evaluated at $\mu = \mu(T=0)$.

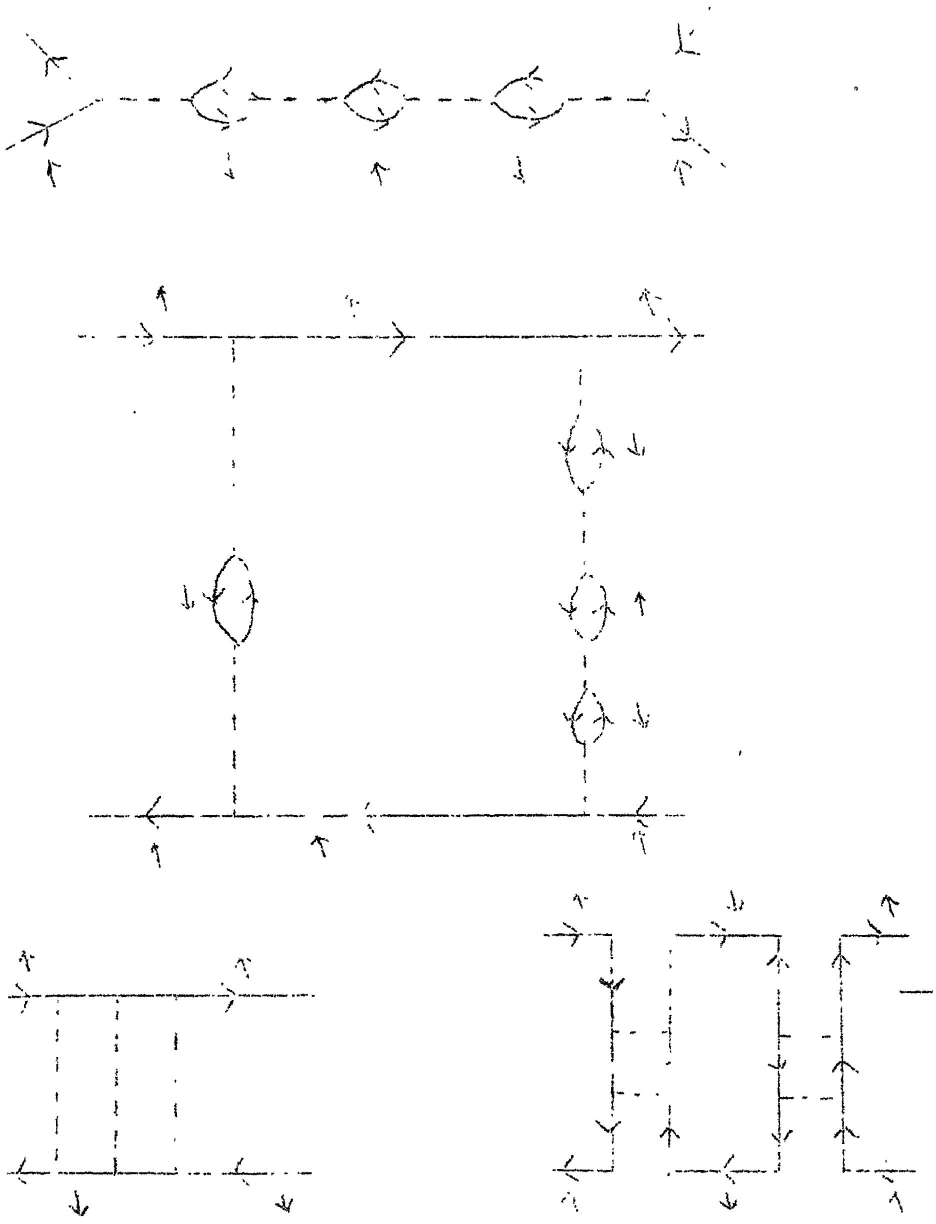


Fig. 10. Diagrams for $\partial^2 \Delta F/\partial B^2$.

An expression for $\chi(T)$ follows quite clearly. Notice that there is no $T^2 \ln T$ term though there is such a term in the specific heat (Eqn. 17, Ref. 13), which is associated with the paramagnon contribution to the single particle self energy (see next Chapter).

Recently, Kawabata[21], using the paramagnon model diagrams of Ma, Beal-Monod and Fredkin,[51] plus the correction due to the renormalisation of the chemical potential due to spin fluctuations, has also obtained the similar results, but with a different numerical coefficient.

If we also express our diagrams in terms of the fermion loops, the lowest order diagrams will look identical to those considered above. Thus at low temperatures, our non-self consistent calculation is identifiable with the paramagnon model. It is futile to argue about the magnitude of coefficient of paramagnon term τ^2/α^2, since it cannot be determined from first principles.

4b. $T^2 \ln T$ term

Barnea uses the expression (we ignore μ_B, etc.)

$$\chi = \left.\frac{\partial M}{\partial B}\right|_{B=0} = \frac{\partial}{\partial B}\left(\langle n_+\rangle - \langle n_-\rangle\right)\Big|_{B=0} \tag{4b.1}$$

where $\langle n_+\rangle$ is calculated in presence of a magnetic field B. Now

$$\langle n_\sigma\rangle = \sum_p G_{p\sigma}$$

and hence

$$\chi = \sum_{p\sigma} \sigma \left(\frac{\partial G_p}{\partial B}\right)_{B=0} \tag{4b.2}$$

The Green's function $G_{p\sigma}$ can be written in terms of the single particle self energy as

$$G_{p\sigma}^{-1} = (\nu_1 - E_{k\sigma}) = \nu_1 - \varepsilon_k + \sigma B - \Sigma_{p\sigma} \tag{4b.3}$$

The $T^2 \ln T$ term comes basically as follows,

$$\frac{\partial G_p}{\partial B} = G_{p\sigma}^2 \left(-\sigma + \frac{\partial \Sigma(p,B)}{\partial B}\right)$$

or $$\sum_{\sigma p} \sigma \frac{\partial G_p}{\partial B} = \sum_{p\sigma} G_{p\sigma}^2 \left(-1 + \sigma \frac{\partial \Sigma_\sigma(p,B)}{\partial B}\right)$$

leading to

$$\chi = -2 \sum_p G_p^2 + \sum_{p\sigma} \sigma \, G_p^2 \left.\frac{\partial \Sigma_\sigma(p,B)}{\partial B}\right|_{B=0} \tag{4b.4}$$

Now consider the first term and expand.

$$G_p^2 = (G_p^{o-1} - \Sigma_p)^{-2}$$

$$= G_p^{o2} + 2\, G_p^{o3}\, \Sigma_p + \ldots .$$

To first order in Σ, this is

$$2 \sum_p G_p^{o3} \Sigma_p$$

$$= 2\sum \left(\frac{1}{\nu_1 - \varepsilon_k}\right)^3 \Sigma_p$$

$$= \sum_p \left\{ \frac{\partial^2}{\partial \varepsilon_k^2} \left(\frac{1}{\nu_1 - \varepsilon_k}\right)\right\} \Sigma_p$$

$$= \sum_{\vec{k}} \frac{\partial^2 f_{\vec{k}}}{\partial \varepsilon_{\vec{k}}^2} \operatorname{Re} \Sigma(\varepsilon_{\vec{k}}, \vec{k}) + \ldots .$$

Since $\mathrm{Re}\Sigma$ contains a term $\tilde{\varepsilon}_k^{\,2} \ln (\tilde{\varepsilon}_k/\varepsilon_f)$, this will obviously contribute a $T^2 \ln T$ term to the susceptibility. And a similar term arises from the second part (of Eq. 4b.4). This is the basis of Barnea's claim.

We now show that there is a cancellation between the two parts, and hence that there is no $T^2 \ln T$ term.

The magnetisation can be obtained from free energy as

$$M = \langle n_+ \rangle - \langle n_- \rangle = \frac{\partial \Delta F}{\partial B} .$$

Consider Fig. 5b for ΔF. Differentiating this with respect to B leads to diagrams (Fig. 11), which can be written as

$$\frac{\partial \Delta F}{\partial B} = \sum_{\underline{p}} \left(G^2_{\underline{p}\uparrow} \Sigma_{\underline{p}\downarrow} - G^2_{\underline{p}\downarrow} \Sigma_{\underline{p}\uparrow} \right) \tag{4b.5}$$

$$= \sum_{\underline{p}\underline{q}} \left\{ G^2_{p\uparrow} G_{p+q\downarrow} \frac{U^2}{1 - U\chi_q^{o+-}} - G^2_{\underline{p}\downarrow} G_{\underline{p}+q\uparrow} \frac{U^2}{1 - U\chi^{o+-}_{\underline{q}}} \right\}$$

$$= \sum_{\underline{q}} \left(-\frac{\partial \chi^{o+-}}{\partial B} \right) \frac{U^2}{1 - U\chi_q^{o+-}} . \tag{4b.6}$$

Differentiating (4b.5) with respect to B once more, gives a term for the susceptibility which is

$$\sum_{\underline{p}} \left(G^3_{\underline{p}} \Sigma^1_{\underline{p}} + G^2_{\underline{p}} \left. \frac{\partial \Sigma^1_{\underline{p}}}{\partial B} \right|_{B=0} \right) . \tag{4b.7}$$

If we look at the either term in (4b.7) separately, we will see a $T^2 \ln T$ term. However, the differentiation of

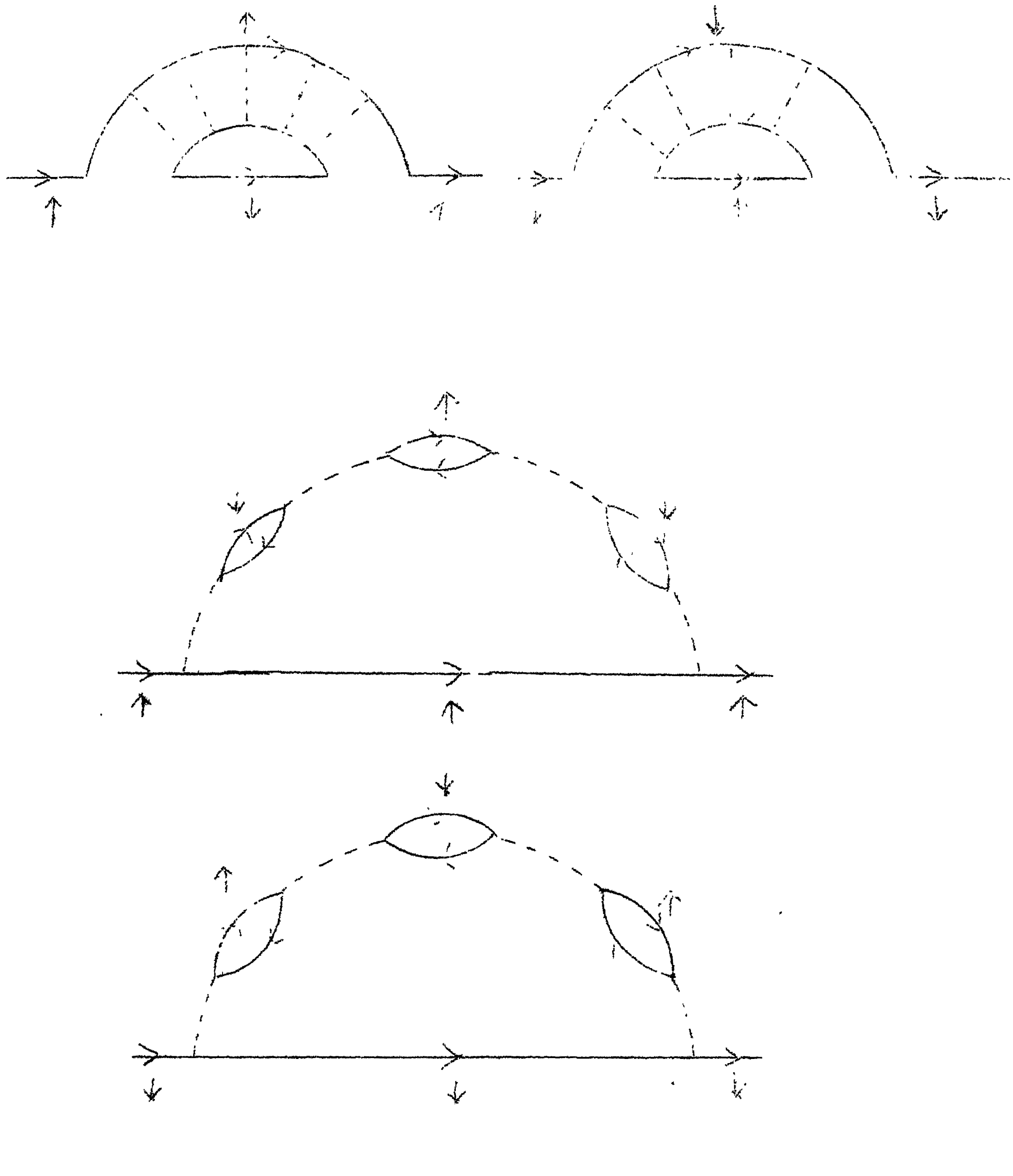


Fig. 11. Diagrams for $\partial\Delta F/\partial B$.

Eqn. (4b.6) leads to

$$(\Delta\chi)^1 = \sum_q \left(\frac{\partial^2 \chi^{o+-}}{\partial B^2}\right) \frac{U^2}{1 - U\chi^{o+-}}$$

$$+ \left(\frac{\partial\chi^{o+-}}{\partial B}\right)^2 \frac{U^3}{(1 - U\chi^{o+-})^2} ,$$

neither of which has a $T^2 \ln T$ term. Since the diagrams considered by us reduce to those of Beal-Monod et al. at low temperatures, this conclusion remains valid in our theory also. The main point is that a $T^2 \ln T$ term does not appear in a spin conserving approximation for χ as is obtained by taking the second derivative of free energy in a magnetic field (Beal-Monod et al.) or an explicitly rotationally invariant approximation (as done by us, with a vector $\vec{\xi}$). The conclusion is true for finite range interaction also. Brinkman and Engelsberg[52] have used $U_o - bq^2$ for $U(q)$; the q^2 term will lead to a term higher order in temperature but no $T^2 \ln T$ term.

CHAPTER III

SPECIFIC HEAT

1. Introduction

The specific heat is perhaps one of the most important thermal properties of condensed matter, since its variation with temperature gives first hand information about low lying excitations and their spectrum. The T^3 behaviour due to Debye phonons, the Dulong-Petit relation and a linear relation for the degenerate Fermi gas are a few examples. We discuss here the effect of spin and density fluctuations on the specific heat of liquid He^3, again a very 'clean' and interesting case. Specific heat in the normal phase of liquid Helium-3 exhibits a quite interesting temperature dependence. For low temperatures ($T << T_F^o \simeq 5°K$) one expects a degenerate Fermi liquid like behaviour with temperature corrections of order $(T/T_F^o)^2$. The observed behaviour is different. The following characteristic features are observed experimentally:[31]

(i) at very low temperatures ($T < 125\ m^ok$), C_V/RT decreases with temperature. The observed behaviour can be written in the form $C_V/RT = a-bT$, a function quite alien

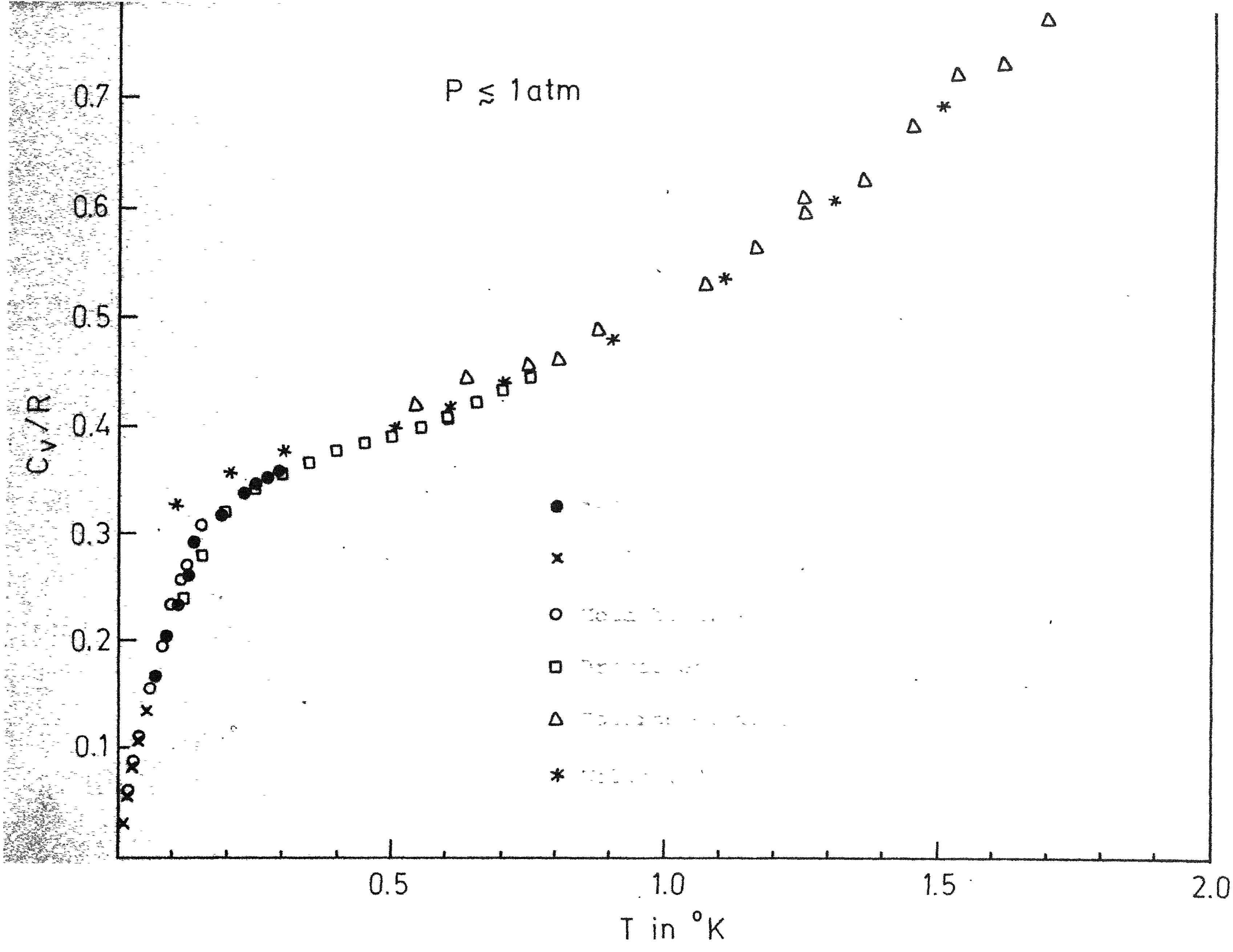


Fig. 12 - Cv/R observed (low pressure).

to Fermi liquid theory. The slope b increases with density. The curve can also be fitted well with a $T^2 \ln T$ term due to paramagnons, but only over a relatively smaller temperature range[53] ($50 < T < 100$ m°k).

(ii) in the intermediate temperature range C_v increases almost linearly upto 0.15°K and then shows a plateau.

(iii) above 1°K, it again starts rising linearly with a slope of nearly $\frac{\pi^2}{4T_F^o} R$ which is half the expected value for a free Fermi gas.

All these features are clearly shown in Fig. 12.

Theoretical calculations can be put mainly into two categories. The one formulated by Goldstein[54] is an effort to explain the intermediate and high temperature behaviour. Here the total entropy of the system is partitioned into two components, the spin entropy and that due to all other degrees of freedom. Through the definition of susceptibility, Goldstein writes an expression for the spin entropy as

$$S_\sigma(T) = \frac{\chi(T)}{\chi_c^o(T)} R \ln 2 \qquad (1.1)$$

with $\chi_c^o(T)$ being the limiting Curie susceptibility and $\chi(T)$ the measured value. The final result for $C_\sigma(T)$ is

remainder is associated with non spin degrees of freedom. Nothing is said about the source of and the temperature dependence associated with the non spin degrees of freedom. Thus the theory is phenomenological and merely relates in a phenomenological model the thermal and magnetic properties of the liquid through an effective "ideal gas magnetic degeneration temperature" and asserts that the spin interaction of the real liquid is accounted for by the empirical ratio $\chi(T)/\chi_c^o(T)$.

The other category consists of theories trying to explain very low temperature behaviour, viz., Landau theory of Fermi liquid, its finite temperature extension and the paramagnon theory. The Landau theory of Fermi liquid[55] is based on the description of interacting Fermi systems in terms of quasi particles. It is assumed that the low lying excitation (quasi-particle) spectrum of a Fermi liquid has a structure similar to that of an ideal Fermi gas. The interaction between quasi-particles can be described through a self consistent field, acting on a quasi particle and produced by the surrounding quasi-particles. The energy of the system will no longer be equal to the sum of energies of separate quasi particles; instead, it is a functional of their distribution function. $E\{n(k)\}$. For calculation of specific heat one starts with the familiar expression for the entropy, viz.,

$$S = - \sum_{\vec{k}\sigma} n_{\vec{k}} \ln n_{\vec{k}} + (1 - n_{\vec{k}}) \ln (1 - n_{\vec{k}}) \quad . \qquad (1.2)$$

This formula has a purely combinatorial origin, and its applicability to a Fermi liquid is determined by the fact that the classification of the quasi-particle levels corresponds by hypothesis to the classification of the particle levels in an ideal gas. For low temperatures where very few quasi particles are excited, the complicated functional eqn. can be simplified and usual procedure for calculating C_v is followed leading to

$$C_v = \frac{1}{3} m^* k_f k_B^2 T \qquad (1.3)$$

here m* is the effective mass at the Fermi surface: a parameter related to the quasi particle interaction function. The eqn. (1.3) gives a linear dependence of the sp. heat on temperature, but experimentally C_V/T never reaches a constant value.

This peculiar behaviour of the specific heat led to the conjecture that terms of the form $T^3 \ln T$ were present in the specific heat. In the microscopic Landau theory, using crossing relations for the vertex part and ward identities, Amit and his associates[56] have shown that these $T^3 \ln T$ terms are related to non-analytic term of the type $|\varepsilon_p - \mu|^3$ in the inverse quasi particle life time τ_p^{-1}, which is a general feature of all normal

Fermi systems and is a consequence of quasi particle interaction $f_{\vec{k},\vec{k}+\vec{q}}$ having a contribution of the form $(\hat{k}.\hat{q})^2$ in the limit $\vec{q} \to 0$. This term also leads to $(k-k_f)^3 \ln |k-k_f|$ term in the quasi particle energy. The physical process responsible for this term is the repeated scattering of a quasi particle-quasi hole pair. In nearly ferromagnetic systems this scattering is particularly large and this is what produces significantly large results.

Using the single particle self energy $\Sigma(\vec{k},\varepsilon_k)$ arising from emission and absorption of paramagnons,[10,11] Berk, Schrieffer and others have calculated the quasi particle entropy from the Fermi distribution $n(\varepsilon_{\vec{k}})$ where $\varepsilon_{\vec{k}}$ includes the self energy $\Sigma(\vec{k},\varepsilon_{\vec{k}})$. This also gives a $T^3 \ln T$ contribution to C_v. Riedel[57] has shown, in full propagator renormalized RPA, that the above procedure gave only part of the $T^3 \ln T$ term in the specific heat. In addition to this part (the 'Fermi' contribution), there are remaining terms which look like the contribution from a system of bosons, although they arise from the fermion degrees of freedom.

Recently, Pethick and Carneiro[58] have remarked that in Riedel's calculation the entropy to order $T^3 \ln T$ is expressed as a sum of dynamical quasi particle contribution (coming from the poles of the single particle propagator) and the Bose contribution coming from the

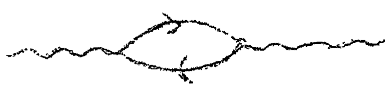
particle hole continuum. However, Balian and de Dominicis[59] and Luttinger[60] have established that the entropy is given by the quasi particle expression evaluated using statistical quasi particle energies. This indicates that Riedel's Bose contribution may be regarded equally well as being due to the difference between statistical and dynamical quasi particle energies.

These theories explain the low temperature behaviour qualitatively but there is controvercy about various origins of the $T^2 \ln T$ term obtained. Moreover, there does not exist any first principle theory which attempts to explain the variation through out the temperature range. In this chapter we analyze the effect of spin and density fluctuations on $C_V(T)$. These are the only excitations liquid Helium-3 supports at low temperatures. We observe that the 'plateau' is due to the Schottky peak like behaviour of the contribution due to the spin fluctuation excitations while the slope $\frac{\pi^2}{4} \frac{1}{T_F^o} R$, at high temperatures is due to suppression of density fluctuation excitations throughout the temperature range. It will also be shown that the 'Bose' and the 'Fermi' terms, both are incorporated in the calculations.

In the next two sections we calculate the contribution due to spin and density fluctuations using our functional integration procedure and then compare our results with the experimental observations on Liq He^3.

2. A Fluctuation Interaction Model

In this section we study $C_V(T)$ in the fluctuation interaction model developed in the previous chapter. We expand $Y[f, \vec{\xi}]$ in even powers of f_α and $\vec{\xi}_\alpha$. odd power terms are zero because of Furry's theorem.[61] The lowest order in ξ



gives RPA for the thermodynamic potential.

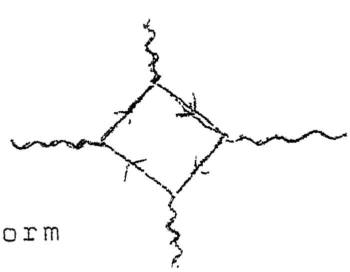
$$\frac{Z}{Z_0} = e^{-\beta(\Omega - \Omega_0)} = \int \left(\Pi_{\alpha i} \frac{d\ \xi_i}{\pi}\right) \exp\left\{-3 \sum_\alpha |\xi_\alpha|^2 \left(1 - U\chi^0_{\underline{q}}\right)\right\}$$

and

$$\Delta\Omega = -\frac{3}{\beta} \sum_{\vec{q}, z_m} \log\left(1 - U\chi^0_{\underline{q}}\right).$$

This in the low temperature limit reproduces the paramagnon results, i.e. a mass enhancement and a $T^3 \ln T$ term for the specific heat.

The next order involves diagrams with four external fluctuation lines, which



Contributes a term of the form

$$\sum_{\underline{q}_1\underline{q}_2\underline{q}_3} K^a_{\underline{q}_1\underline{q}_2\underline{q}_3} \vec{\xi}_{\underline{q}_1} \cdot \vec{\xi}_{\underline{q}_2} \vec{\xi}_{\underline{q}_3} \cdot \vec{\xi}_{-(\underline{q}_1+\underline{q}_2+\underline{q}_3)}$$

$$+ K^b_{\underline{q}_1\underline{q}_2\underline{q}_3} \vec{\xi}_{\underline{q}_1} \cdot \vec{\xi}_{\underline{q}_2} f^*_{\underline{q}_3} f_{-(\underline{q}_1+\underline{q}_2+\underline{q}_3)}$$

+ pure f term.

The first term gives coupling between four spin fluctuations while the second denotes coupling between the density and spin fluctuations*. Similarly, the higher order diagrams can be drawn and the expression written. Thus effectively we have a system of coupled anharmonic oscillators with a wave vector and frequency dependent coupling. Obviously, as such the problem is highly intractable and one has to rely upon some drastic but plausible approximations. Let us begin with the fourth order. First of all we assume the coupling coefficients K's to be $\vec{q}$ and ω independent. This assumption has already been discussed earlier and amounts physically to performing an average over 'fast' Fermion degrees of freedom and retaining the 'slow' SF variables and assuming the SF coupling to be local. Next consider the coupling with density fluctuations. We average over the 'density' degrees of freedom, this gives

$$\sum_{q,q_1} K^b \langle f_q^* f_q \rangle \quad \xi_{q_1}^* \, \xi_{q_1}$$

This type of averages $\langle f^*f \rangle$ are discussed in the next section. The general result is that because of the density fluctuation suppression the average has a temperature dependence, far milder than the free Fermi gas term, i.e. $\tau^2/U_{eff}\,\rho_{\epsilon_F} \ll \tau^2$. This will effectively renormalize the

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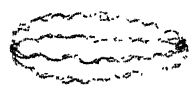
* The coefficients K^a and K^b are written in terms of the product of four fermion propagators.

'harmonic' force constant, but with no extra temperature corrections.

Next consider the quartic term in SF. Obviously, the standard method is to work in the quasi harmonic approximation, that is, write x^4 as $\langle x^2 \rangle x^2$ and then estimate the error thus introduced. Doing this the terms of the form

$$K_1^a < |\xi^-_{-\underline{q}}|^2 > \quad \xi^{z*} \; \xi^z, \; K_2^a \quad < |\xi^z_{-\underline{q}}|^2 > \quad \xi^{+*} \; \xi^+$$

etc. are obtained. These averages have already been calculated in the previous chapter. Thus upto quartic term in the quasi harmonic approximation the problem is solved. We have neglected the difference $[<\xi^4> - <\xi^2> \; <\xi^2>]$ which arises from fluctuation correlation effects, e.g., from diagrams  , where the wavy lines represent fluctuation propagators. The distinctive thermal parts of these can be shown to be of nonleading order in temperature. We can improve our approximation somewhat by putting in the true or observed susceptibility where averages $\mathop{\mathrm{Lt.}}_{\underline{q}\to 0} < \xi_{\underline{q}} \; \xi_{-\underline{q}} >$ appear. Thus we work in a quasi-harmonic approximation for the spin fluctuation excitations.

In the paramagnetic phase $< |\xi^z_{\underline{q}}|^2 > \; = \; < |\xi^+_{\underline{q}}|^2 >$ and we can write the change in thermodynamic potential due to spin fluctuations as

$$\Delta\Omega = - \frac{3}{\beta} \sum_{\underline{q}} \ln \left(1 - U \; \chi^o(\underline{q}) \; + \lambda \frac{1}{\beta} \sum_{\underline{q}'} D(\underline{q}')\right) \qquad (2.1a)$$

$$= \; -3/\beta \sum_{\underline{q}} \ln \left(\chi_p / \chi(\underline{q}) \right) \; . \qquad (2.1b)$$

After performing the frequency summation one can partition the resultant integral into a zero temperature and a thermal part. Because of its weak temperature dependence we omit the zero temperature part. Its contribution to specific heat (linear term) is assumed to be small. The thermal part is given by

$$\Delta\Omega = -\frac{6}{\pi} \sum_{q} \int_{0}^{\infty} \tan^{-1} \left(\frac{\gamma\pi\omega/qv_f}{1 - U\chi^{o}(q,0) + \frac{\lambda}{\beta}\sum_{\underline{q}'} D^{t}(\underline{q}')} \right) \left(\frac{1}{e^{\beta\omega} - 1} \right) \tag{2.2}$$

The denominator in the argument of $\tan^{-1}$ function is nothing but the static susceptibility, $\chi^{-1}_{(q')}$, calculated in the one spin fluctuation approximation. (One can improve the results, introducing higher order correlation in χ^{-1} also. While performing the numerical calculations we substitute experimental numbers for $\chi(0,0)$, which obviously takes all correlations into account.) $\Delta\Omega$ depends on temperature through the Bose factor and the temperature dependence of $\chi^{t}(0,0)$. The latter have already been calculated in the paramagnon and the Curie limit. Thus one can get an explicit expression for $\Delta\Omega(T)$. The energy integration can be performed exactly,[48] giving

$$\Delta\Omega = -\frac{6}{\beta} \sum_{\vec{q}} [\log\Gamma(x) - (x-\tfrac{1}{2})\ln x + x - \tfrac{1}{2}\ln 2\pi] \tag{2.3}$$

where

$$x = \frac{qv_f}{2\pi^2\gamma k_B T(\chi^{t}_{q}(0)/\chi^{o}_{q})} \backsimeq \frac{qv_f(\alpha(T) + \delta q^2)}{2\pi^2\gamma k_B T}\,. \tag{2.4}$$

Specific heat can now be calculated using the relation

$$\Delta C_v = -T \frac{\partial^2 \Delta \Omega}{\partial T^2} ,$$

giving

$$\frac{\Delta C_v}{k_B T} = 6T \sum_{\vec{q}} \{ (\frac{2}{T} \frac{\partial x}{\partial T} + \frac{\partial^2 x}{\partial T^2}) \phi(x) + (\frac{\partial x}{\partial T})^2 \phi'(x) \} \qquad (2.5)$$

where $\phi(x) = \psi(x) + \frac{1}{2x} - \ln x$.

With $\phi(x) = \frac{-1}{2x + 12x^2}$ and x given by equation (2.4) one can perform the momentum integration numerically. But an analytic estimation of $C_v(T)$ in various temperature regimes is possible. For this one needs $\alpha(T)$ which has already been calculated. $\alpha(T)$ enters the expression with its various temperature derivatives as

$$\frac{\Delta C_v}{k_B T} = \sum_{\vec{q}} \{ \mu_{\vec{q}} \phi(x) \frac{\partial^2 \alpha}{\partial T^2} + \mu_{\vec{q}}^2 \frac{1}{T} \phi'(x) (\frac{\partial \alpha}{\partial T} - \frac{\alpha + \delta q^2}{T})^2 \} \qquad 2.6)$$

(i) Very low temperatures $\tau << \alpha_o$: Here $\alpha(T)$ is given by its paramagnon limit form, i.e. $\alpha(T) \sim \alpha_o + A \frac{\tau^2}{\alpha_o}$ and since $x >> 1$, $\phi(x)$ can be approximated as

$$\phi(x) = - \frac{1}{12x^2}$$

with this and observing that α' and α'' won't contribute to the leading temperature dependence we find

$$\frac{\Delta C_v}{k_B T} \sim \sum_{\vec{q}} \frac{1}{\mu_q (\alpha + \delta q^2)} . \qquad (2.7)$$

which yields $\Delta C_v \sim T \ln (1/\alpha_o)$, the standard paramagnon mass enhancement contribution. Next higher order terms can be obtained by using a series expansion for $\phi(x)$ in this regime, i.e.

$$\phi(x) = -\frac{1}{12x^2} + \frac{1}{120x^4} - \frac{1}{252x^6} \cdots ,$$

and the first term gives a $T^3 \ln T$ contribution. The coefficient is calculated as below:

$$\frac{C_v}{6k_BT} \simeq \frac{1}{T} \sum_q \mu_q^2 \left(-\frac{1}{30}\right) \frac{1}{x^5} \frac{x^2}{\mu_q^2}$$

$$\sim -\frac{1}{30} \frac{1}{T} \frac{4\pi}{(2\pi)^3} \qquad \frac{(2\pi^2 \gamma k_BT)^3 \, q^2 \, dq}{q^3 v_f^3 (\alpha + \delta q^2)^3}$$

$$\sim -\frac{4\pi}{30} \frac{(2\pi^2\gamma k_B)^3}{(2\pi)^3 v_f^3} T^2 \int_{q_c}^{\infty} \frac{dq}{q(\alpha + \delta q^2)^3} \qquad (2.7)$$

where $q_c = \dfrac{2\pi^2 \gamma k_B T}{\alpha_o v_f}$, the low cutoff in this limit. The integration is trivial and the most significant term is $\frac{1}{2} \frac{1}{\alpha_o^3} \ln \frac{\alpha_o}{\tau^2}$, which leads to a $T^3 \ln T$ contribution to specific heat. This term has been obtained by many authors. Later in this section we will show that both 'Bose' and 'Fermi' terms are incorporated in our calculation. Thus we get a $T^3 \ln T$ term in specific heat but no such term in the susceptibility $\chi(T)$. The same result is obtained by Beal-Monod et al.[13] for paramagnon model.

(ii) The intermediate temperature ($\tau < 1$): Here $\alpha(T) \sim T/T_F^{\,o}$, the 'Curie' behaviour. And $\phi(x) \sim -\frac{1}{2x}$ since $x < 1$. With these, $C_v(T)$ can be calculated as below. At these temperatures, $\alpha(T)\ \alpha T$ so that $\frac{\partial^2 \alpha}{\partial T^2} = 0$ and $\frac{\partial \alpha_{q=0}(T)}{\partial T} = \frac{\alpha_{q=0}(T)}{T}$. Using these relations in Eq. (2.6) and $\phi(x) \sim -\frac{1}{2x}$, we see that we are left with a very small term for C_v behaving basically as $(1/T^2)$ (Eq. 2.2) Going back to $\Delta\Omega$, we find that in this regime, $\Delta\Omega \sim k_B T$ so that $\Delta C_v \sim 0$. So the extra specific heat goes to nearly zero.

Thus because of spin fluctuations and their correlations specific heat has an interesting temperature dependence. At low temperature it has a dominant paramagnon like behaviour and increases to a maximum and then falls off as $1/T^2$. The numerical results are discussed in the next section.

Now we check whether the $T^3 \ln T$ term obtained here incorporates both the 'Bose' and the 'Fermi' contribution. Let us consider the RPA expression for the thermodynamic potential,[52]

$$\Delta\Omega = \frac{1}{\beta} \sum_{\underline{q}} \left[\ln\left(1 - U\chi^o{}_{\underline{q}}\right) + U\chi^o{}_{\underline{q}}\right]$$

$$= \sum_{\vec{q}} \int_c \frac{d\omega}{2\pi i}\, g(\omega) \left[\ln\left(1 - U\chi^o{}_{\underline{q}}\right) + U\chi^o{}_{\underline{q}}\right], \qquad (3.9)$$

the contour encircles the real axis from $-\infty$ to ∞ in the clockwise direction, omitting the pole of $g(\omega)$ at $\omega=0$. Here $g(\omega)$ is the Bose function. The shift of entropy is given by

$$\Delta S_T = -\frac{\partial \Delta\Omega T}{\partial T}$$

$$= -\sum_{\vec{q}} \int_c \frac{d\omega}{2\pi i} \frac{\partial g(\omega)}{\partial T} [\ln (1-U\chi^o_{\underline{q}}) + U\chi^o_{\underline{q}}]$$

$$- \sum_{\vec{q}} \int_c \frac{d\omega}{2\pi i} g(\omega) \frac{\partial}{\partial T} [\ln (1-U\chi^o_{q}) + U\chi^o_{\underline{q}}] \qquad (3.10)$$

Carrying out the temperature differentiation in the second term and performing the contour integration, we obtain for this term

$$\sum_{\vec{q}} U^2 \int_{-\infty}^{\infty} \frac{d\omega}{\pi} g(\omega) \quad m\ \chi^{-+}(\vec{q},\omega)$$

$$\times \sum_{\vec{k}} \left(\frac{\partial f_k}{\partial T} - \frac{\partial f_{k-q}}{\partial T}\right) \frac{P}{\omega - \varepsilon_k + \varepsilon_{k-q}}$$

$$- \sum_{\vec{k}\,\vec{q}} U^2\ g(\varepsilon_k - \varepsilon_{k-q})\ \mathrm{Re}\ \chi^{-+}(\vec{q}, \varepsilon_k - \varepsilon_{k-q})$$

$$\left(\frac{\partial f_k}{\partial T} - \frac{\partial f_{k-q}}{\partial T}\right) \qquad (3.11)$$

Now we use the identity

$$g(\varepsilon_k - \varepsilon_{k-q}) \left\{\frac{\partial f_k}{\partial T} - \frac{\partial f_{k-q}}{\partial T}\right\}$$

$$= -\frac{\partial}{\partial T}\left[f_{\vec{k}} (1 - f_{\vec{k}-\vec{q}}) - (f_{\vec{k}} - f_{\vec{k}-\vec{q}}) \left(\frac{\partial}{\partial T} g(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}-\vec{q}})\right)\right],$$

(3.12)

and rewrite the equation (3.11). Doing contour integral in the first term in (3.10) and combining equations (3.12), (3.11) and (3.1?):

$$\Delta S_T = \sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\partial g(\omega)}{\partial T} \left[\tan^{-1} \frac{U\chi_I^0(\vec{q},\omega)}{1-U\chi_I^0(\vec{q},\omega)} - \frac{U\chi_I^0(\vec{q},\omega)\,(1 - U\chi^0_R(\vec{q},\omega))}{(1-U\chi^0_R(\vec{q},\omega))^2+(U\chi^0_I(\vec{q},\omega))^2}\right]$$

$$- \sum_{\vec{k}} \frac{\partial f_{k\sigma}}{\partial T} \; \mathrm{Re} \; \Sigma_\sigma^T(\vec{k}, \varepsilon_{\vec{k}\sigma}) \qquad (3.13)$$

χ^0_I and χ^0_R are the real and imaginary parts of χ^0 when $\omega = \omega + i0$. Notice that there are two thermal contributions coming from equation (3.13). One form $\frac{\partial g(\omega)}{\partial T}$, the Boson contribution and the second from the thermal part of the fermion self energies. Fermion self energies are given by

$$\Sigma_\uparrow^T(\vec{k}, \varepsilon_{\vec{k}\downarrow}) = -U^2 \sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\mathrm{Im}\,\chi^{-+}(\vec{q},\omega)}{\omega-\varepsilon_{k\uparrow}+\varepsilon_{k-q\downarrow}} (g(\omega)+1-f_{k-q\downarrow})$$

and $$\Sigma_\downarrow^T(\vec{k}, \varepsilon_{\vec{k}\downarrow}) = U^2 \sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\mathrm{Im}\,\chi^{-+}(\vec{q},\omega)}{\omega-\varepsilon_{k-q\uparrow}+\varepsilon_{k\downarrow}} (g(\omega) + f_{k-q\uparrow}).$$

In the paramagnetic phase, we use

$$\mathrm{Im}\,\chi^{-+}(\vec{q},\omega) = -\,\mathrm{Im}\,\chi^{-+}(\vec{q},-\omega)$$

to write

$$\Sigma^T_{\uparrow}(\vec{k},\varepsilon_{\vec{k}}) = \Sigma^T_{\downarrow}(\vec{k},\varepsilon_{\vec{k}})$$

$$= U^2 \int_0^\infty \frac{d\omega}{\pi} \, \mathrm{Im}\, \chi^{-+}(\vec{q},\omega) \left[\frac{f_{\vec{k}-\vec{q}}+g(\omega)}{\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}+\vec{q}}+\omega} + \frac{1-f_{\vec{k}-\vec{q}}+g(\omega)}{\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}-\vec{q}}-\omega} \right] . \tag{3.14}$$

This is the self energy contribution coming from the diagram (Fig. 11). Thus both the Fermi and Bose terms for ΔS are contained in our expression which reduces to (3.9) for low T.

3. Density Fluctuations

At low temperatures the Fermi liquid supports density oscillations also. These oscillations can be generated by coupling a scalar probe to the density. The excitation spectrum consists of single pair, multipair and collective oscillations. For low frequencies ($\omega < qv_f$) single pair excitations share most of the spectral density while for the high frequency ($\omega > qv_f$) a collective mode occurs as a resonance over an almost uniform spectrum of the multi pair excitations. For a charged Fermi liquid the collective mode is plasmon mode while for a neutral Fermi liquid (e.g. Liq He^3) it is zero sound. All these excitations contribute to the free energy and therefore to temperature dependence of specific heat. We again work in the functional integral scheme. To the lowest order, density fluctuations can be considered to be independent of SF. The density fluctuation contribution in 'RPA' is

$$e^{-\beta\Omega} = \int \frac{d^2 f_{\underline{q}}}{\pi} \; e^{-\sum_{\underline{q}} |f_{\underline{q}}|^2 (1 + V\chi^o_{\underline{q}})}$$

or
$$\Omega = k_B T \sum_{\underline{q}} \ln (1 + V\chi^o_{\underline{q}})^{-1} . \qquad (3.1)$$

This is the interaction part, since it goes to zero as $V \to 0$. To this we should add a 'free' part. Consider

$$e^{-\beta\Omega_o} = \int \frac{d^2 f_{\underline{q}}}{\pi} \; e^{-\Sigma |f_{\underline{q}}|^2 (\rho_{\varepsilon_f} / \chi^o_{\underline{q}})}$$

This gives

$$\langle f_{\underline{q}}^{\;2} \rangle = \langle \rho_{\underline{q}} \; \rho_{-\underline{q}} \rangle = \frac{\chi^o_{\underline{q}}}{\rho_{\varepsilon_f}}$$

i.e., correct 'free' susceptibility in units of ρ_{ε_F}.
Therefore in this approximation

$$\Omega_o = k_B T \sum_{\underline{q}} \ln \left(\frac{\chi^o_{\underline{q}}}{\rho_{\varepsilon_f}}\right). \qquad (3.2)$$

This gives a T^2 term in Ω_o which with proper q_c adjustment reproduces the free Fermi gas value. For V very large (3.1) nearly cancels (3.2) and the remaining contribution to the specific heat is very small in comparison to free Fermi gas value. This can be shown as follows. The equation (3.1) can be rewritten

$$\Omega = -\frac{1}{\pi} \sum_{\vec{q}} \int \frac{d\omega}{e^{\beta\omega}-1} \tan^{-1} \left\{ \frac{V \, I_m \, \chi^o_{\vec{q}}(\omega)}{1 + VRe \; \chi^o_{\vec{q}}(\omega)} \right\} , \qquad (3.3)$$

We have just converted the frequency sum to an integral. For low temperatures $k_B T \sim \omega \ll \varepsilon_f$ and $\omega < qv_f$; $\tan^{-1} x$ can be

expanded as power series in its argument and to the lowest order the contribution to specific heat is reduced by a factor $\sim (V\rho_{\varepsilon_F})$, as can be seen on adding (3.2) and (3.3). The exact size of this reduction can be obtained as follows. Clearly the density susceptibility

$$\underset{\vec{q}\to 0}{\mathrm{Lt.}} \langle \rho_{\vec{q}}\ \rho_{-\vec{q}} \rangle = \left(\frac{1}{1 + V\rho_{\varepsilon_F}}\right) \langle \rho_{\vec{q}}\rho_{-\vec{q}} \rangle_{free}$$

and this is simply the (compressibility) bar numerical factors. The latter is known, e.g. from sound velocity. For example, the first sound velocity is $(S^1_{true}/S^1_{free})^2$ ~ 5.0 (at 0.28 atm.) and ~ 13.0 (at 27 atm.). Thus, one has, respectively, $(1+V\rho_{\varepsilon_F}) = 5$ and $(1+V\rho_{\varepsilon_F}) = 14$. Expanding the total contribution of density fluctuations to Ω as a power series in $(V\rho_{\varepsilon_F})^{-1}$, we find that with these value of $(V\rho_{\varepsilon_F})$, the free fermion contribution $\frac{\pi^2\tau}{4}$ is reduced by factors of 5 and 13 respectively. Physically the reason for this reduction is clear. The He^3 fluid is relatively incompressible; compared to a free fermi gas the smallest q (longest wavelength, lowest energy) density fluctuation require excitation energies higher by a factor of five to fourteen. Thus these excitations contribute only a small fraction of the free fermi gas value to C_v, and in the first approximation can be ignored throughout the degenerate fermi gas range. At intermediate temperatures,

$(T \gtrsim 1°K)$, we are left with only the 'free' spin fluctuation term (the sf interaction term goes to zero as $1/T^2$) i.e. $\pi^2 \tau/4$. This is indeed observed.

4. Comparison with Experiment

We describe here a calculation of $C_v(T)$ for liquid He^3, based on the above theory. According to this theory, the specific heat can be written as a sum of three terms; $C_v(T) = C_v^{o\ s.f.}(T) + \Delta C_v^{s.f.}(T) + C_v^{d.f.}(T)$. The first is the free or noninteracting spin fluctuation term $C_v^{o\ s.f.}(T)$ whose value is $\frac{1}{2} C_v^{free}(T) = \frac{\pi^2}{4} \frac{T}{T_F^o} = (\pi^2 \tau/4)$. The latter result can be proved by expressing the change of the free fermion gas energy with temperature T $(\ll T_F^o)$ in terms of density and spin fluctuation excitations with respect to the (zero temperature) ground state. Both of these contribute equally. Then there is the extra contribution $C_v^{s.f.}(T)$ due to low lying spin fluctuation excitations. This has been calculated above (section 3.2, Eq. 2.5) in a quasi-harmonic approximation which retains the leading temperature dependent terms. The third is the density fluctuation term which, we have argued above (section 3) is smaller than the free fermi gas value $\frac{\pi^2 \tau}{4}$ by a factor of nearly five (low density) to thirteen (high density). The separation of specific heat into additive contributions from spin and

density fluctuations is not exact; clearly there is coupling between them. This coupling basically renormalizes in a temperature independent way fluctuation interaction vertices and propagators. These cannot be accurately calculated anyway (see Chapter II, sections 2b,2c for details). Because of the smallness of the density fluctuation term, we take it, as a first approximation, to be zero. The extra fluctuation interaction term $\Delta C_v(T)$ goes to zero for $T \gg \alpha T_F^0$, so that in this range, if our assumption regarding $C_v^{d.f.}(T)$ is correct, we expect

$$C_v(T) \cong C_v^{o\ s.f.}(T) = \frac{\pi^2}{4}\left(\frac{T}{T_F^o}\right) = \frac{\pi^2\tau}{4} .$$

An examination of the data, e.g. for low pressures or density ($P \lesssim 1$ atm.) shows (see Fig. 17) that this is indeed true. Above $T \simeq 1°K$, the $C_v(T)$ curve is a straight line, and the slope $\frac{C_v(T)}{\tau} = 2.3 \simeq \frac{\pi^2}{4}$. We thus subtract this term from the observed $C_v(T)$ and exhibit the difference, i.e. $C_v^{s.f.}(T)$ in units of R as a function of reduced temperature $\tau = (T/T_F^o)$. Fig. 13 shows the experimental points for low pressure and Fig. 14 shows them for high pressure. We note the relatively steep (enhanced) initially linear rise. $C_v(T)$ peaks at a rather low temperature ($\tau_{peak} \simeq 0.025$), definitely less by a factor of two or three than α_o, the obvious characteristic dimensionless spin fluctuation temperature. Further, the peak position

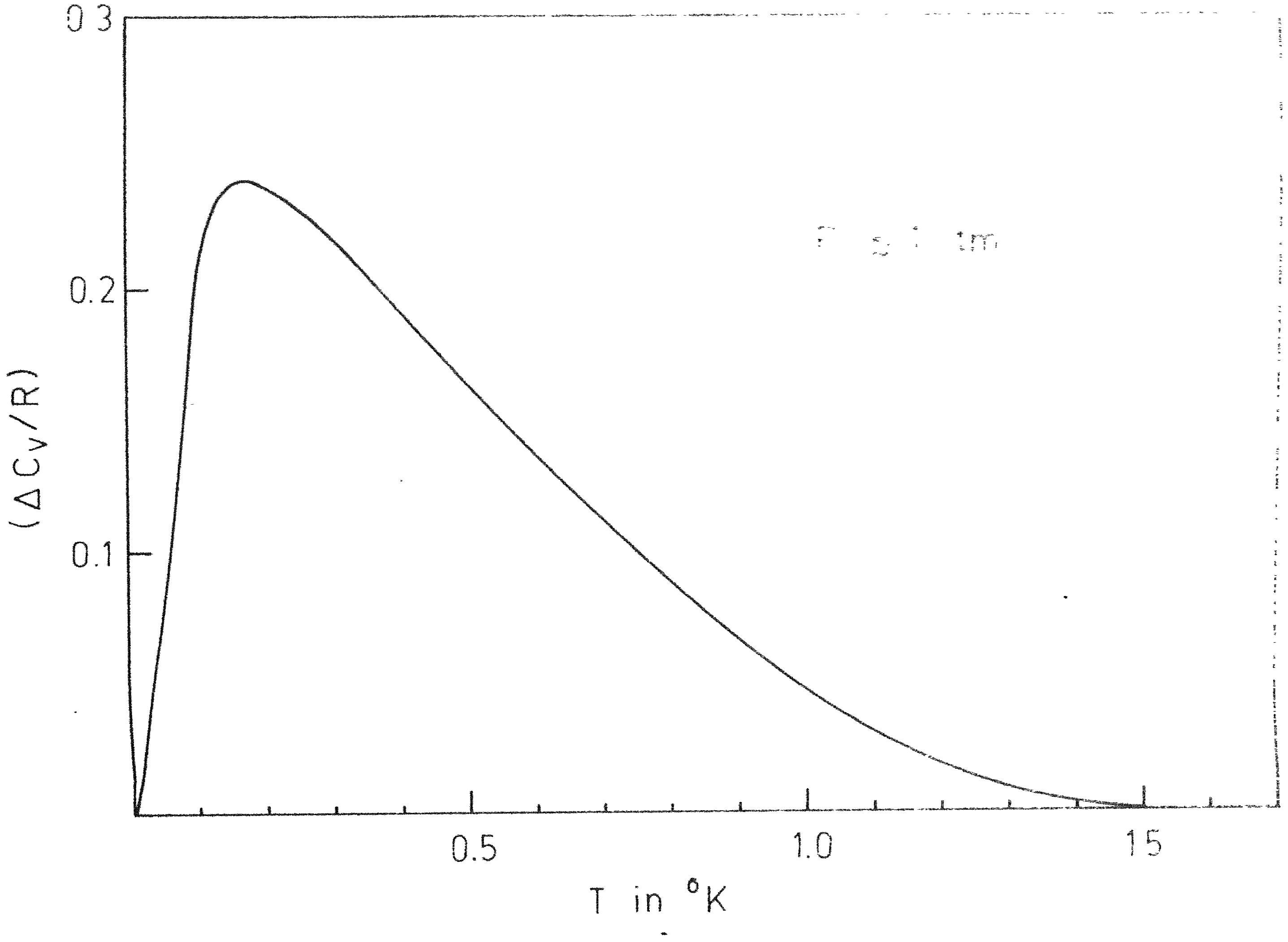


Fig. 13 - Experimental $\Delta C_V/R$ vs T for liquid H_e^3 (low density).

and the peak value do not (within experimental error) shift very much between the low and high density limits. Certainly they do not relate linearly to α_o. The value of $(\Delta C_v/R)$ at the peak is ~ 0.25; the peak is rather small. After the peak $C_v(T)$ decreases rather slowly but continuously and the decrease is parabolic in the tail region.

The expression, Eq. (2.5), is found to reproduce the broad features of the observed $C_v(T)$ curve correctly in every case. One input information required is the susceptibility inverse, $\alpha(T)$, and its first and second derivatives. We take these from experiment. Obviously, there is some inaccuracy in the first derivative, and considerably more in the second derivative. We have tried to do the best possible by a least squares fit to both the observed values and the theoretical numbers. We also need the 'free' fermi temperature T_F^o. While in actuality the spin fluctuation coupling falls off rapidly with increasing q, in our zero range model it does not. We thus have to suitably cut off the contribution from large q fluctuations. This we do by a simple cutoff q_c, which is the only free parameter in the theory. The actual numbers obtained depend significantly on the cutoff. This is understandable, since the thermodynamic potential is not very strongly affected by just the small q fluctuations. For example,

at low temperature, $\Delta\Omega \sim \tau^2 \ln(1 - U\chi^o_q)$. Thus the $q \simeq 0$ fluctuations for which $1-U\chi^o_q \simeq \alpha_o \ll 1$ do contribute significantly more, but this contribution falls off gently with q. We first report features which do not depend on the cutoff, and then a calculation with a particular cutoff which gives good agreement with experiment.

For a wide range of q_c values between $0.5k_F$ to $1.5k_F$, we find that the initial nearly linear rise, the peaking at a low temperature, and the slow fall off beyond the peak are reproduced. As q_c varies from $0.5k_F$ to $1.5\ k_F$, the initial slope increases, the peak position shifts from $=0.015$ to 0.030, and the peak value from $\frac{\Delta C_v}{R} \sim 0.15$ to 0.40 (all in the high density case). The fall-off beyond the peak is slow, and the rate is in all cases comparable with experiment. As an example, we show in Fig. 14, $C_v^{s.f.}(T)$ with $q_c = 1.1k_F$ (high density He^3, $T_F^o = 6.18°K$). We used the Lindhard $\chi^o_{\vec{q}}$ here; for this q_c, there is actually very little difference between this and the small q form used in calculating $\chi(T)$. We see that the initial increase, the peak position, the peak height all agree accurately with experiment. The falloff after the peak is a little faster than experiment. The overall agreement is good.

The general experimental features of $C_v^{s.f.}(T)$ may be summarized as follows. In the classical regime $\tau > \alpha_o$,

the spin susceptibility is Curie like, i.e. like that of a zero temperature ferromagnet. As analyzed by Murata and Doniach,[14] $C_v(T)$ for itinerant fermion ferromagnets above T_c rises (due to classical spin fluctuation effects) on approaching T_c. This is seen, for example, in $ZrZn_2$. In our case, the rise is smothered by quantum effects which reduce the entropy and C_v, and require (for a normal fermi system) that $C_v(T) \to T$ as $T \to 0$.

CHAPTER IV

ZERO TEMPERATURE FERROMAGNET

In this short chapter, an interlude, we discuss a hypothetical (?) case. a ferromagnet with $T_c = 0°K$. This can be realized in principle if the pressure on the system (Liq He^3) is increased enormously (corresponding to $T_F^o \sim 6.8°K$), and if it is prevented from solidifying. Here we discuss only the spin susceptibility. In the second chapter we have seen that in the temperature range $\alpha_o < \tau << 1$, the spin susceptibility behaves as

$$\chi = \frac{\chi_p}{\alpha(T)} \simeq \frac{\mu_B^2}{a\alpha_o + T} .$$

That is, like a collection of classical spins. We are observing a classical behaviour for a highly degenerate fermi system. Spin fluctuations have pushed the system into a classical regime as far as the magnetic properties are concerned. This feature gets revealed very clearly if we put $\alpha_o = 0$ in the expression for susceptibility and solve the equation self consistently. As $\alpha_o \rightarrow 0$, the paramagnon regime ($\tau << \alpha_o$) gets narrower and a 'classical' behaviour is expected down to zero degree Kelvin. When

such a calculation is performed we get a universal curve and the calculated susceptibilities for $\alpha_o \neq 0$ tend asymptotically towards this.

This is a very interesting case. Here we are effectively calculating the susceptibility of a ferromagnet with $T_c = 0$. The quantity of interest, obviously is the critical exponent. The effect of spin fluctuation correlation on critical behaviour for finite T_c ferromagnets has been discussed by Ramakrishnan.[18] In the present case, in contrast to a non-zero T_c ferromagnet MFFA gives the correct critical behaviour. The reason is the following. Suppose for $\alpha_o = 0$, $\alpha(T) \sim \tau^{\lambda}$. Then the non classical (paramagnon) region $\tau/\alpha << 1$ means $\tau^{1-\lambda} << 1$ and occurs only if $\lambda < 1$. This is not possible and so one always has the other (Curie-Weiss) region. Here the spin fluctuation correlation term is of the form (Eqn. (2c.9) of Chapter II).

$$\tau^2 \ln (1/\alpha) \sim \tau^2 \ln (1/\tau)^{\lambda} << \tau^{\lambda} .$$

If $\lambda \sim 1$, the correlation term never becomes more important than the mean fluctuation field term.

To calculate the index λ, notice that theoretically for small α_o

$$\alpha = \frac{AT}{\delta} \{q_c - (\frac{\alpha}{\delta})^{1/2} \tan^{-1} q_c \sqrt{\delta/\alpha}\}$$

as $\alpha_o \to 0$, $\alpha(T) \simeq \frac{AT}{\delta} q_c$. As such q_c goes as $T^{1/3}$ but

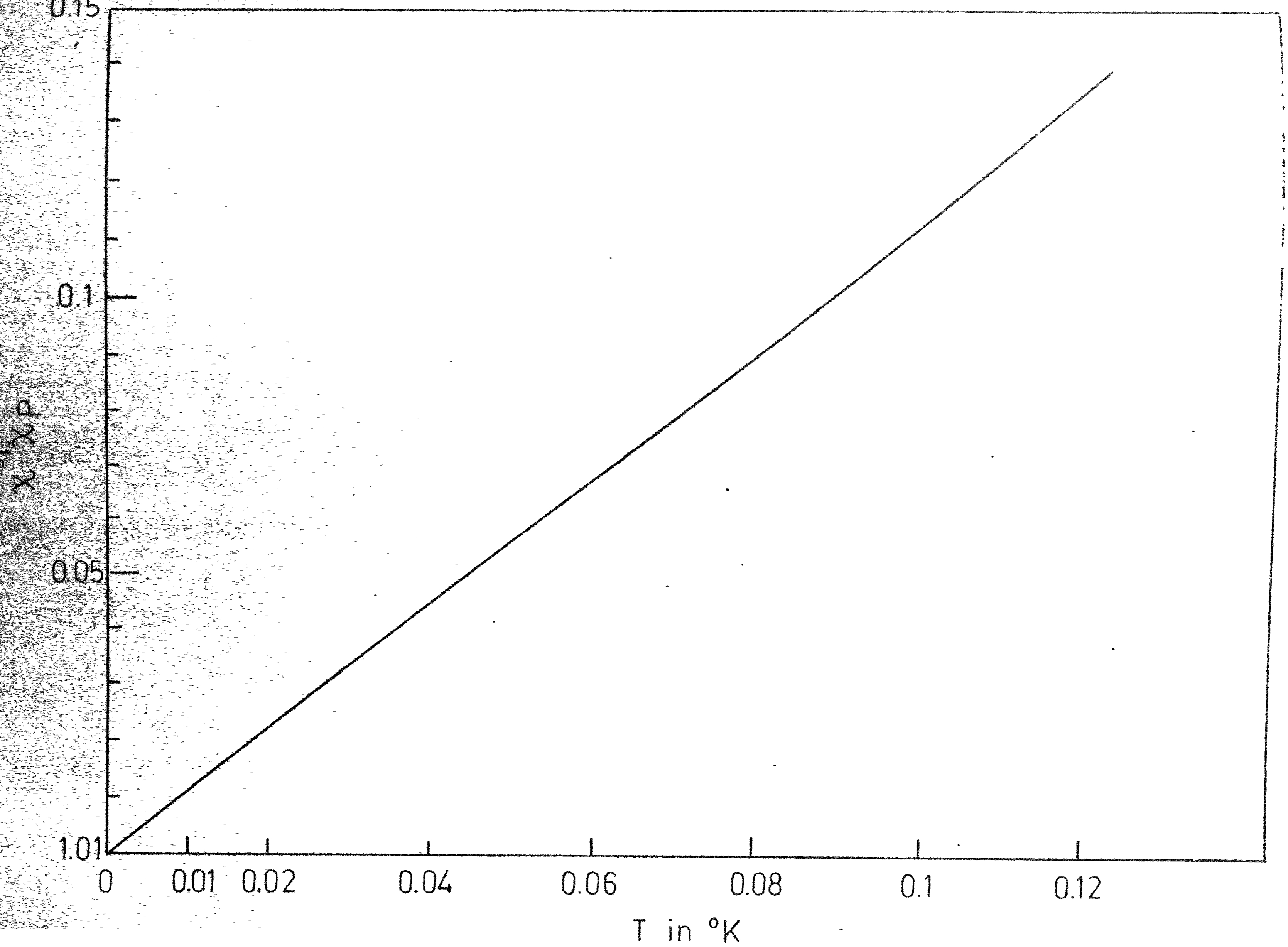


Fig. 15. $\chi^{-1}\chi_P$ vs. τ for a $T_C = 0$ ferromagnet.

because of small δ one can safely put $\lambda \propto T$. This is what one expects for a purely classical system.

We have calculated $\alpha(T)$ in a self consistent two spin fluctuation approximation. The parameter Λ_1 is chosen to be that of high density case. A linear variation of α is obtained (Fig. 15) giving $\lambda = 1$, for the critical exponent. The effective Curie constant is nearly the same as that of a free spin 1/2 system of the same density.

A similar conclusion has been obtained by Hertz[23] who has discussed the problem using renormalization group methods. The new feature in this problem is the fact that because of the Bose factor $(e^{\beta\omega} - 1)^{-1}$, the number of thermal (classical) fluctuations becomes smaller and smaller as $T \to 0$ (i.e. as the critical point is approached). This reduces the phase space for fluctuation correlations. In the RNG analysis, this requires the introduction of a suitably scaled 'energy' variable as a degree of freedom additional to the three momentum variables q_x, q_y and q_z. In effect, the dimensionality increases by one, and therefore the behaviour is mean field like $(d = 3+1 = 4)$. We see this explicitly in our procedure of calculating fluctuation correlation corrections perturbatively. The perturbation method converges, the leading correction going to zero

($m_s \to 1$) since the effect of electronic energy changes on magnetization is large. There is no small expansion parameter.

In weak itinerant ferromagnets $T_c << T_F$. There are systems, e.g. $ZrZn_2$,[65] Ni_3Ga,[33] Ni-Pt,[26] and Ni-Pd[66] alloys which have magnetization much smaller (in units of μ_B) than the number of holes per atom. One can again ask the basic question. What are low lying excitations in this system and how do they couple to magnetization. In the Stoner theory these are electron-hole excitations. They decrease the molecular field via the thermal occupation effect.[65,67,68] At low temperatures an unenhanced T^2 term, $\Delta m = (T^2/T_F^2)m = \tau^2 m$ is obtained. The next step is to consider the collective longitudinal and transverse spin fluctuation excitations. The former are overdamped, resonant excitations and have characteristic energy (for low q) $\sim m^2 \epsilon_F$. The latter are well defined collective modes (poles) with dispersion $\omega = Dq^2$, up to a cutoff ω_c and then a resonance part. While the importance of these excitation for m(T) has been recognized,[15,22] there exists no systematic study of these effects. In this chapter we show that there is an enhanced T^2 effect and a reduced $T^{3/2}$ term for Δm at low temperatures. Near T_c, a 'classical' mean field behaviour is obtained.

Since expressing the free energy and its derivatives as functionals of the spin fluctuations $\vec{\xi}_q$ (Chapters II and III) is an order parameter (Ginzburg Landau) approach, its extension to the ferromagnetic case is obvious. We separate out the mode ξ^z_{oo} which is macroscopically occupied, and after integrating over all other s.f. modes and over fermion degrees of freedom, express the free energy as a function of ξ^z_{oo} (henceforth abbreviated as ξ_o). For small values of ξ_o (weak ferromagnet) a power series expansion of $F(\xi_o)$ in which the first few terms are retained is expected to be sufficient. The coefficients of ξ_o^n in such an expansion contain the effect of the integrated out degrees of freedom, namely (coupled) spin fluctuations. The characteristic temperature dependences are present therein. However, this programme cannot be carried out here as it stands since as we shall see $F(\xi_o)$ depends on ξ_o in a nonanalytic way. In particular, there is a term τ^2 in ξ_o arising from the effect of incoherent longitudinal and transverse spin fluctuations, and a term $\sim(\tau\xi_o)^{3/2}$ arising the spin wave (magnon) excitations. Because of this, we adopt a somewhat different approach where we directly evaluate the equilibrium value of ξ_o, i.e. we evaluate $(\frac{\partial F}{\partial \xi_o})$ and equate it to zero to obtain $\xi_o^{eq.} = \xi(T)$. $(\frac{\partial F}{\partial \xi_o})$ can be written in the form, $\xi_o - B\{<n_\uparrow>_{\xi_o} - <n_\downarrow>_{\xi_o}\}$

where α is a constant and $\langle n_\sigma \rangle$ is the average number of electrons of spin σ. We include the thermal effect of spin fluctuations and spin waves to leading order while calculating $\langle n_\sigma \rangle$. Further, since ξ_0 is small, we expand in powers of ξ_0 wherever permissible, and retain only the leading significant terms. The method and results obtained are discussed in the subsequent sections.

Next we study the magnetisation $m(H,T)$ in a magnetic field. Here, Wohlfarth et al.[26] have shown, by analyzing a GL like model with a Stoner-Wohlfarth temperature dependence for $m(T)$, that the Arrott plot of $m^2(H,T)$ against $H/m(H,T)$ should be a straight line. Experimental plots (e.g. in Ni-Pt alloys) show a systematic departure for small H/M and large temperatures. We obtain the Arrott plot expression in a GL-like scheme retaining s.f. effects, and find such a deviation.

2. Fluctuation Interaction Theory

The ferromagnetic phase is characterised by a non-zero value for the order parameter (the spontaneous magnetisation). The presence of this long range magnetic order enters through the special importance of the time and space averaged longitudinal fluctuation field ξ^z_{00} which plays the role of a molecular field. We use the fluctuation interaction theory discussed in Chapter II and modify

it to treat the effect of ξ^z_{oo} ($\equiv \xi_o$) exactly in the fermion as well as the fluctuation propagators. The other fields ξ^+, ξ^- and $\xi^z_{q\neq 0, u\neq 0}$ will then be treated in the Gaussian approximation. This effectively amounts to inclusion of fluctuation effects in fermion self energy to lowest order.

To treat the effect of ξ^z_{oo} exactly we split the z-component of the fluctuation field as

$$\xi^z_{\vec{q},u} = \xi^z_{o,o} + \tilde{\xi}^z_{\vec{q},u} \tag{2.1}$$

where

$$\xi^z_{oo} = \frac{1}{\beta} \sum_{\vec{q}} \int_0^\beta du\, \xi^z_{\vec{q},u}$$

then

$$\frac{1}{\beta} \sum_{\vec{q}} \int_0^\beta du\, |\xi^z_{\vec{q}u}|^2 = {\xi^z_{oo}}^2 + \frac{1}{\beta} \sum_{\vec{q}} \int_0^\beta du\, |\tilde{\xi}^z_{\vec{q}u}|^2 \tag{2.2}$$

From here onwards we denote $\tilde{\xi}^z_{\vec{q}u}$ by $\xi^z_{\vec{q}u}$ and ξ^z_{oo} by ξ_o. Now the expression (Eqn. (2a.11) Chapter II, dropping d.f. variables, f_α) for the partition function can be transformed to one involving effect of ξ_o explicitly. This is done by transforming the statistical average with respect to an unperturbed density matrix to an average with respect to the density matrix inwhich the molecular field (ξ_o) effects are included in the Hamiltonian exactly. The result is

$$\frac{Z}{Z_o} = \int_{-\infty}^{\infty} \frac{d\xi_o}{\sqrt{\pi}}\, e^{-\xi_o^2}\, Z_{static}(\xi_o) \times$$

$$\times \int \prod_\alpha \frac{d^2\vec{\xi}_\alpha}{\pi^3} \exp\{-Y[\vec{\xi}_\alpha]_{\xi_o,0}\} \tag{2.3}$$

where

$$\mathcal{L}_{\text{static}}(\xi_0) = \langle T_u \{\exp[-\int_0^\beta c^z S_q^z (u')\ \xi_0\ du']\}\rangle \tag{2.4}$$

while $Y[\vec{\xi}_\alpha]_{\xi_{0,0}}$ is calculated in the Heisenberg representation of $(H_0 - 2c^z\ \xi_0\ S^z)$. This has the effect of changing the single particle energy from ε_k to $E_{k\pm} = (\varepsilon_k \mp c^z\ \xi_0)$, i.e. there is a spontaneous magnetic field. Moreover, the fluctuation propagators will also depend on ξ_0 and hence the longitudinal and the transverse propagators will not be identical.

We are interested in the free energy difference between the para and ferromagnetic phases. Notice that, to the lowest order in temperature the free energy is equal to μN (N = total no. of particles), plus the Ω evaluated at $\mu(T=0)$. The proof is easy: let $\mu + \delta\mu$ be the chemical potential at temp T; then

$$\begin{aligned} F &= \Omega(\mu + \delta\mu,\ T) + (\mu + \delta\mu)\ N \\ &\cong \Omega(\mu, T) + (\frac{\partial\Omega}{\partial\mu} + N)\ \delta\mu + \mu N \\ &= \Omega(\mu, T) + \mu N, \end{aligned}$$

since $N = -\dfrac{\partial\Omega}{\partial\mu}$. μN is constant in temperature and plays no role in discussion. Thus one should not consider the temperature dependent μ shift while evaluating F, and should work with $\mu(T=0)$. We can now replace the thermodynamic potential Ω by free energy F (plus a constant).

...w if an integration over all variables except ξ_0 is ...rformed, we get ... a function depending on ξ_0 ...ly. That is, ... equation (2.3) can formally be written as

$$...^{-\beta ...} \cdot \int_{-\infty}^{\infty} \frac{d\xi_0}{\sqrt{\pi}} e^{-G(\xi_0)}$$

where

$$G(\xi_0) = \xi_0^{2} + \beta F_{static}(\xi_0) + \beta F_{S.F.}(\xi_0).$$

The minimization condition

$$\left. \frac{\partial G(\xi_0)}{\partial \xi_0} \right|_{\xi_0 = \xi} = 0 \qquad (2.5a)$$

or $\quad 2\xi + \beta F'_{static}(\xi) + \beta F'_{SF}(\xi) = 0 \qquad (2.5b)$

gives $\xi(T)$. To obtain $\xi(T)$ from (2.5b), one can proceed directly, namely develop a systematic approximation for $F_{SF}(\xi_0)$ ($F_{static}(\xi_0)$ can be calculated exactly) and then find the field derivative. We find it easier to write down an alternative version of (2.5a), and to examine the effect of spin fluctuations etc. on the quantity $\{\langle n_\uparrow\rangle - \langle n_\downarrow\rangle\}$ occurring in that equation. ξ_0 occurs in the exponent of $\frac{Z}{Z_0}$ (see e.g., Eq. (2.4)) in two places. Firstly, there is the Gaussian term ξ_0^{2}. Secondly, there is an additional term in the single particle energy: $-\xi_0 c^{z} \sum_k (a^\dagger_{\vec{k}\uparrow} a_{\vec{k}\uparrow} - a^\dagger_{\vec{k}\downarrow} a_{\vec{k}\downarrow})$. Thus, it is directly clear that

$$\frac{\partial G(\xi}{\partial \xi_0} = 0 \Rightarrow 2\xi_0 - \beta c^z < \sum_k (a^\dagger_{k\uparrow} a_{k\uparrow} - a^\dagger_{k\downarrow} a_{k\downarrow}) >_{\xi_0} = 0 \tag{2.6a}$$

$$\text{i.e.} \quad 2\xi_0 - \beta c^z (<n_\uparrow>_{\xi_0} - <n_\downarrow>_0) = 0 \tag{2.6b}$$

This result is expected since ξ_0 is magnetization order parameter variable. We discuss below how the equilibrium $\xi(T)$ is calculated from Eq. (2.6).

3. Magnetization

We see from Eq. (2.6) that the effect of spin fluctuations and spin waves on ξ_0 is contained in their effect on the single particle propagator G_p. Quite generally, one can write

$$G_{\underline{p}\pm} = \frac{1}{G^{0-1}_{\underline{p}} \pm c^z \xi_0 - \Sigma_{\underline{p}\pm}} \tag{3.1}$$

In eq. (3.1), $\Sigma_{\underline{p}\pm}$ is to be calculated in the presence of of the molecular field ξ_0, and of coupling between the fermion and spin fluctuation variables (see for example, Eq. 2a.6, Chapter II). The usual diagrammatic rules (Appendix II) are used. Clearly, $\Sigma_{\underline{p}\pm}$ can be expressed in terms of spin fluctuation propagators and fermion variables. The simplest approximation for $\Sigma_{\underline{p}}$, describing the effect of coupling with one spin fluctuation, is

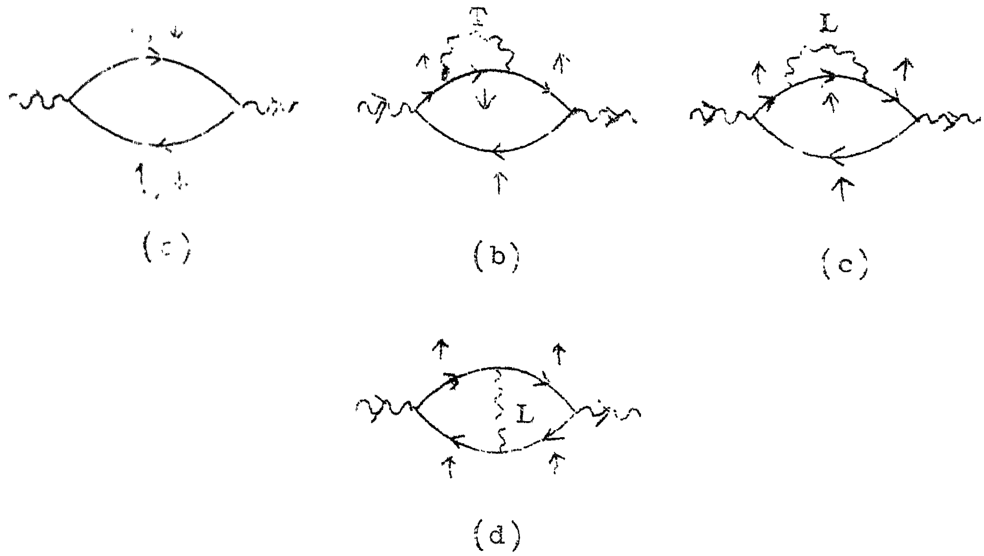


Fig. 17. The fluctuation propagator D^L.
(a) RPA contribution; (b), (c), (d) one spin fluctuation contributions (D^T and D^L).

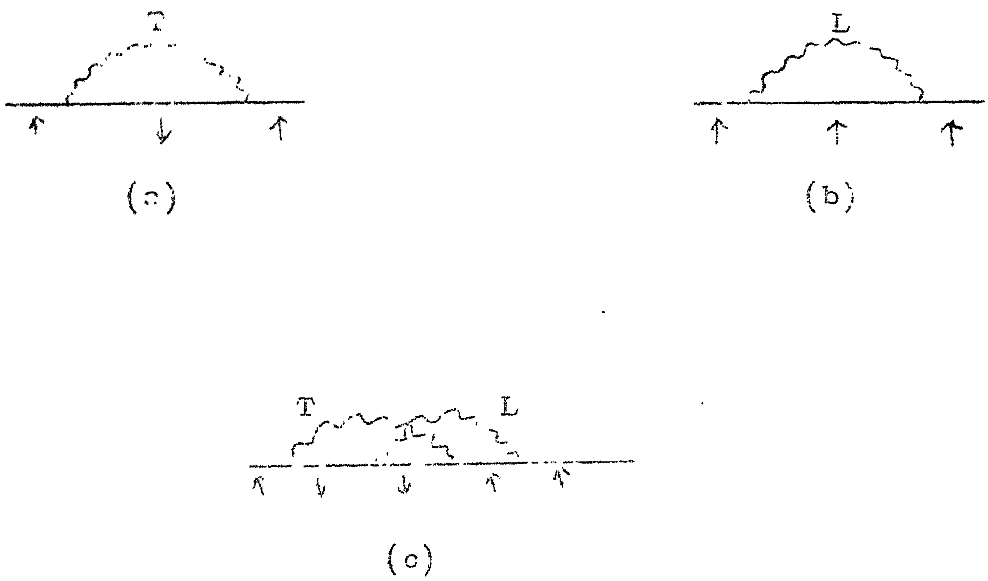


Fig. 16. (a), (b) Fluctuation contribution to single particle energies.
(c) Higher order diagram.

shown in Fig. 16. Here the wavy line is a transverse or longitudinal spin fluctuation propagator. We find

$$\Sigma_{\underline{p}\pm} = \frac{1}{\beta} \sum_{\underline{p}'} D^T (\underline{p}-\underline{p}', \xi_o) G_{\underline{p}'\mp}$$

$$+ \frac{1}{\beta} \sum_{\underline{p}'} D^L (\underline{p}-\underline{p}', \xi_o) G_{\underline{p}'\pm} \tag{3.2}$$

In terms of $\Sigma_{\underline{p}\pm}$, $\langle n_\uparrow \rangle_{\xi_o} - \langle n_\downarrow \rangle_{\xi_o}$ can be written as

$$\langle n_\uparrow \rangle_{\xi_o} - \langle n_\downarrow \rangle_{\xi_o} =$$

$$- 2\sqrt{\frac{U}{\beta}}\, \xi_o \left(\frac{1}{\beta} \sum_{\underline{p}} G_{\underline{p}}^{o2}\right) - 2 \left(\frac{U}{\beta}\right)^{3/2} \xi_o^{\ 3} \left(\frac{1}{\beta} \sum_{\underline{p}} G_{\underline{p}}^{o4}\right) \tag{3.3a}$$

$$+ \frac{1}{\beta} \sum_{\underline{p}} G_{\underline{p}}^{o2} (\Sigma_{\underline{p}+} - \Sigma_{\underline{p}-}) \tag{3.3b}$$

$$- 2\sqrt{\frac{U}{\beta}}\, \xi_o \left[\frac{1}{\beta} \sum_{\underline{p}} G_{\underline{p}}^{o3} (\Sigma_{\underline{p}+} + \Sigma_{\underline{p}-})\right] . \tag{3.3c}$$

In writing equation (3.3), we have expanded $\langle n_\uparrow \rangle_{\xi_o} - \langle n_\downarrow \rangle_{\xi_o}$ as a power series in Σ and have kept only the first non-vanishing term. This is because the leading temperature dependent effect is given by this term. Terms quadratic and higher in Σ have temperature dependent parts going as higher powers of T (see Chapter II, section 2b for an analysis of this kind of thing), and can be neglected. Further, since ξ_o is small* we have expanded the regular

---

* ξ_o is macroscopic, of order $\sqrt{N}$, so that $\xi_o^{\ 2} \sim O(N)$. There however need be no apprehension that we expand in powers of $\sqrt{N}$. Our free energy is well behaved (proportional to N), and the actual expansion parameter is $\xi_o/\sqrt{N}$, a quantity

[illegible] $\left(\sum_{p} \frac{1}{\epsilon_p^{n-1} \pm c^z \xi_o}\right)$ as a power series in ξ_o, and have [illegible] terms cubic in ξ_o. This should be sufficient for [illegible] ferromagnets. We remark that terms (3.3.) and (3.3) need not be well behaved as functions of ξ_o, we shall find that they are not. So what we have here is a mixed fluctuation amplitude and ξ_o expansion.

It can be shown that the new temperature dependences which arise from more complicated self energy diagrams (see e.g., Fig. 16) are stronger (higher powers of τ) and hence negligible for $\tau \ll 1$ (the case considered here). This is not true close to T_c as we approach T_c from below. There the spin fluctuation correlation diagrams become important, and our approximations (3.3) and (3.2) for $\langle n_\uparrow \rangle - \langle n_\downarrow \rangle$ break down. This critical region is rather small for weak ferromagnets. A perturbative estimate of its width[18] is $|\tau_c - \tau| \sim e^{-1/\tau_c}$ where $\tau_c = (T_c/T_F^o)$ is the dimensionless critical temperature.

Footnote (...Contd.)

of order N^o, and for weak ferromagnets, $\ll 1$. For reference, we give below the N dependence of various quantities occurring earlier and later in this chapter :-

$\xi_o \sim \sqrt{N}$, $\langle n_\uparrow \rangle - \langle n_\downarrow \rangle \sim N$, $D^{T,L}(\xi_o) \sim N$,

$\rho_{\epsilon_F} \sim N$, $\rho''_{\epsilon_F} \sim N$, $U \sim \frac{1}{N}$, $U_4 \sim N^{-2}$.

To actually find the effect of spin fluctuations on ξ_0 in our approximation, we substitute the expression (3.-) for Σ into Eq. (3.3). We make the local spin fluctuation coupling approximation (e.g. writing $\frac{1}{\beta}\sum_{\underline{p}}\sum_{\underline{q}} G_{\underline{p}}^{\,4} D^L(\underline{q},\xi_0) = (\frac{1}{\beta}\sum_{\underline{p}} G_{\underline{p}}^{\,4})(\sum_{\underline{q}} D^L(\underline{q},\xi_0)$; see chapter II, section 2b for a discussion), and find that Eq. (2.6) becomes

$$\xi_0\,(1 - U\rho_{\varepsilon_F}) + \xi_0^{\,3}\,\frac{U^2}{\beta}\,\left(\frac{\rho''_{\varepsilon_F}}{6}\right)$$

$$- \xi_0\, U^2\, \frac{\rho''_{\varepsilon_F}}{6}\,(3D^L(\xi_0) + 2D^T(\xi_0)) = 0 \quad . \qquad (3.4)$$

In terms of the dimensionless (or fractional) magnetization $\frac{1}{2}\langle n_\uparrow\rangle - \langle n_\downarrow\rangle = m = \frac{\xi_0}{\sqrt{U\beta}}$, and the dimensionless quartic fluctuation coupling constant $U_4 = -(\frac{U^3\rho''_{\varepsilon_F}}{6})$, Eq. (3.4) can be written

$$m^2\, U_4 = (U\rho_{\varepsilon_F} - 1) - \frac{U_4}{U}\,[3D^L(\xi_0) + 2D^T(\xi_0)]\,. \qquad (3.5)$$

In Equations (3.4) and (3.5), the transverse and longitudinal fluctuation amplitudes $D^T(\xi_0)$ and $D^L(\xi_0)$ appear. These are

$$D^L(\xi_0) = \frac{1}{\beta}\sum_{\underline{q}} D^L(\underline{q},\xi_0) \qquad (3.6)$$

and $$D^T(\xi_0) = \frac{1}{\beta}\sum_{\underline{q}} D^T(\underline{q},\xi_0)\,. \qquad (3.7)$$

If in equation (3.5), the second term on the right [illegible] (i.e. the fluctuation contribution) is neglected, we [illegible] the Stoner result for the saturation (T=0) magnetization of [illegible] weak ferromagnet, i.e.,

$$m_0^2 = \left(\frac{U\rho_{\varepsilon_F} - 1}{U_4}\right) \qquad (3.8)$$

In the Stoner-Wohlfarth theory, the temperature dependence of m arises from the thermal occupation probability of fermions, i.e. we have, at $T \neq 0$, not $U\rho_{\varepsilon_F}$ but $-U\int f_{\varepsilon}^{-1}\, d\varepsilon$ and thus Eq. (3.8) becomes (for $T \neq 0$)

$$m^2 = \frac{(U\rho_{\varepsilon_F} - 1)}{U_4} + \frac{\pi^2}{6}\,\frac{U}{U_4}\,\rho''_{\varepsilon_F}\,(k_B T)^2$$

$$= m_0^2\left[1 - \frac{T^2}{T_c^2}\right] \qquad (3.9)$$

where $\quad k_B T_c = \frac{m_0 U}{\pi}\,.$ $\qquad (3.10)$

We compare this temperature dependence with that obtained by us later.

In order to compute the temperature dependence of m(T) from Eq. (3.5), we need to know $D^{L,T}(\xi_0)$. Obviously, this cannot be done exactly. From our work earlier, e.g. Chapters II and III, we expect that a one spin fluctuation approximation for the self energies $\Sigma^T(\underline{q}, \xi_0)$ and $\Sigma^L(\underline{q}, \xi_0)$ should be adequate. We discuss this and more refined approximations below (section 4).

[illegible] clear from the foregoing that determination [illegible] involving a complicated self consistency [illegible] depends on D^T and D^L; these in turn depend [illegible] in section 4 that for the weak ferromagnet [illegible], the problem can be solved partly, and at [illegible] temperature dependences in various temperature regimes can be obtained simply.

4. D^L and D^T

A definite approximation scheme for calculation of D^L and D^T in the ordered phase is needed. We have already calculated these for normal phase. There, because of the absence of spontaneous magnetisation and because of the rotational invariance of the Hamiltonian, $D^T = D^L$. This is no longer true. The longitudinal excitations are overdamped, resonant modes while the transverse are long-lived collective modes (spin waves) in a small (ω/ϵ_F, $q/k_f < O(1)$) region of phase space and are resonant modes outside this region. We calculate these propagators in the fluctuation interaction scheme.

To begin with, we consider the propagator D^L. We calculate the self energy Σ^L in an approximation very similar to that used in Chapter II. We retain only the one spin fluctuation term, i.e. in Σ^L, we keep the diagrams describing the coupling of the longitudinal s.f.

... or one transverse spin fluctuation. ... before, to be evaluated selfconsistently. ... earlier, the leading thermal effects are ... in this approximation. The correlated two spin ... temperature dependence is similar and ... a one s.f. term with appropriately ... fficients. In addition, we include the contribution of the molecular field ξ_o to leading order.

... first write down the latter term. This is given diagrammatically by Fig. 17 and has the expression

$$\Sigma^{L}_{HF} = - \frac{U}{2}\frac{1}{\beta} \sum_{\underline{k}} (G^{o}_{\underline{k}\uparrow} G^{o}_{\underline{k}+\underline{q}\downarrow} + G^{o}_{\underline{k}\downarrow} G^{o}_{\underline{k}+\underline{q}\downarrow})$$

$$\simeq U \chi^{o}(\underline{q}) - \frac{3U_4}{U\beta} \xi_o^{\,2} \qquad (4.1)$$

where

$$G^{o}_{\underline{k}\uparrow(\downarrow)} = (\nu_1 - \varepsilon_k + (-) c^z \xi_o)^{-1} . \qquad (4.2)$$

The single particle propagators $G^{o}_{\underline{k}\sigma}$, are evaluated exactly in presence of the field ξ_o. Now assuming the fluctuation vertices to be ξ_o independent, the one s.f. correction term can be written as (Fig.17b,c,d).

$$\Sigma^{L}_{1,s.f.} = - \frac{U_4}{U} (3D^{L}(\xi_o) + 2D^{T}(\xi_o)) \qquad (4.3)$$

We later show how the propagator

$$D^{L}(\underline{q}) = (1 - U\chi^{o}(\underline{q}) + \frac{3U_4}{U\beta} \xi_o^2 + \frac{U_4}{U} (3D^{L}+2D^{T}))^{-1} \qquad (4.4)$$

[illegible] in terms of a relation involving only [illegible]. [illegible] simplifies the problem of self consistency [illegible].

[illegible] arises in approximating D^T similarly. [illegible] propagator has the well known spin wave [illegible] ω [illegible] for small q and ω (in our case of $q < q_c$ $\sim$ [illegible]). [illegible] need not appear in a given approximation for D^T. In fact, the one spin fluctuation approximation for D^T does not lead to a pole (i.e. to $(D^T)^{-1} \to 0$ as $\omega \to$ [illegible] and $\vec{q} \to 0$). We show in the next chapter how, using the Ward identity, one can obtain a spin wave in a scheme where fluctuation effects are included. Here we simply assume that in the pole region, $D^T(\vec{q}, z_m)$ has the standard form

$$D^T(\underline{q}) = \frac{1}{\rho\varepsilon_F} \frac{m(T)}{z_m - Dq^2} \tag{4.5}$$

where the spin wave stiffness D is calculated in the next chapter. In the continuum regime ($q > q_c \sim mk_f$, $\omega > m^2 \varepsilon_f$), $D^T(\underline{q})$ has a broad resonance. Here, ω and q are large enough so that m or m^2 can be treated perturbatively. (This obviously is not to be done in the spin wave or Stoner gap regime). Here we write for D^T (or Σ^T) an expression analogous to that for D^L (or Σ^L); i.e. we include spin fluctuation coupling and coupling to ξ_0 both to leading

... ...imation smoothly goes over to the one ... chapter II where $\xi_o \to 0$. Since in this ... ξ_o ... considered small with respect to ω, q ... expression for D^T is expected to describe the ... temperature dependent behaviour correctly. We ...

$$\Sigma_{\cdot} \;\; - \beta \sum_{\underline{k}} G^{o}_{k\downarrow} G^{o}_{k+q\uparrow}$$

$$- \; \chi^{+-}(\underline{q})$$

$$= \; \chi^{o}(\underline{q}) - \frac{U_4}{U\beta} \;\; \xi_o^{\;2}, \tag{4.6}$$

(the last equation is valid for small ξ_o only), and

$$\Sigma_1^T \; \text{b.f.} \;\; - \frac{U_4}{U} \;\; (D^L(\xi_o) + 4D^T(\xi_o)) \tag{4.7}$$

so that

$$D^T(\underline{q}) = (1 - U\chi^o(\underline{q}) + \frac{U_4}{U\beta}\xi_o^{\;2} + \frac{U_4}{U}(D^L(\xi_o) + 4D^T(\xi_o))^{-1}. \tag{4.8}$$

The equation (3.4) can be used to express D^L in terms of magnetisation only.

$$D^L(q) = [\frac{2U_4}{U\beta}\xi_o^{\;2} - U\;\{\chi^o\;(\underline{q}) - \chi^o(0)\}]^{-1}$$

$$= [\frac{2U_4}{U\beta}\xi_o^{\;2} + \delta q^2 + \frac{i\pi\gamma\omega}{qv_f}]^{-1}. \tag{4.9}$$

This after integration leads to (Refer Chapter II for details),

$$\frac{1}{\rho_{\varepsilon}} \frac{\tau^{2} U \beta}{3 U_4 \xi_0^{2}} = \frac{a}{\rho_{\varepsilon_F}} \frac{\tau^2}{m^2} \quad \text{for } \tau << m^2,$$

or

$$\frac{1}{\rho_{\varepsilon}} \tau^{4/3} \text{ for } \tau > m^2 \tag{4.10}$$

where a and a' are positive constants. Since $m \leq m(T=0)$, the first condition means $\tau << m_o^2 \sim \tau_c$. This holds at low temperatures. The second condition is true only at high τ. As we will see, at high temperatures, $m^2 \sim (\tau_c - \tau)$ and hence this condition means $\tau >> \tau_c - \tau$ or $\tau >> \tau_c/2$. Thus up to $T_c/2$ we expect a T^2 dependence changing over smoothly to a $T^{4/3}$ dependence beyond this.

The effect of transverse fluctuations has been discussed by Yamada[22] also. In the spin wave region he obtains a $T^{3/2}$ and a $T^{5/2}$ term due to spin waves and their interaction with single particle excitations respectively. Using (4.5) and performing the frequency and $\vec{q}$ summation one obtains for the spin wave region,

$$D^T = \frac{1}{\rho_{\varepsilon_F}} m(T) \sum_{\vec{q}} \int \frac{\delta(\omega - Dq^2)}{e^{\beta\omega} - 1} \frac{d\omega}{\pi}$$

$$= \frac{1}{\rho_{\varepsilon_F}} m(T) (k_B T/D)^{3/2}, \tag{4.11}$$

a $(T/T_c)^{3/2}$ contribution reduced by a factor $m(T)$.

In the resonance region ($q > m_o k_f$, $\omega > m_o \varepsilon_f$) D^T is given by Eq. (4.8). It is easily seen that this expression

... that for D^L. We therefore find that

$$\sum \cdot (\ldots) \quad \rho_{\varepsilon_F} \frac{\tau^2}{m^2} \quad \tau \ll m^2$$

$$\rho_{\varepsilon_F} \tau^{4/3} \quad \text{for } \tau > m^2 \tag{4.12}$$

Thus at low temperatures the fluctuation contribution to ... self energy varies as τ^2/ξ_o^2 and hence the terms (3.3b) and (3.3c) are not well behaved functions of ξ_o. Since this behaviour is valid only for $\tau < m^2$, it is ... The same term gives a contribution $\tau^2 \ln \xi_o$ to free energy and hence the Ginzburg Landau expansion in powers of ξ does not hold at very low temperatures. At high temperatures ($\tau \simeq \tau_c$), this term does not exist and the expansion is valid as usual.

We conclude this section by summarizing the broad features. In the low temperature region the equation (3.4) reads

$$m^2(T) = m_o^2 \left(1 - \alpha \frac{\tau^2}{m^2 m_o^2}\right) - m \left(\frac{\tau}{m_o}\right)^{3/2} \tag{4.13}$$

That is, there is an enhanced τ^2 (just like in X(T) for highly paramagnetic fermi liquids) and a reduced $\tau^{3/2}$ contribution due to spin fluctuations at low temperatures $\tau < \tau_c/2$. At high temperatures (near T_c),

$$m^2 = \tau_c^{4/3} - \tau^{4/3} \tag{4.14}$$

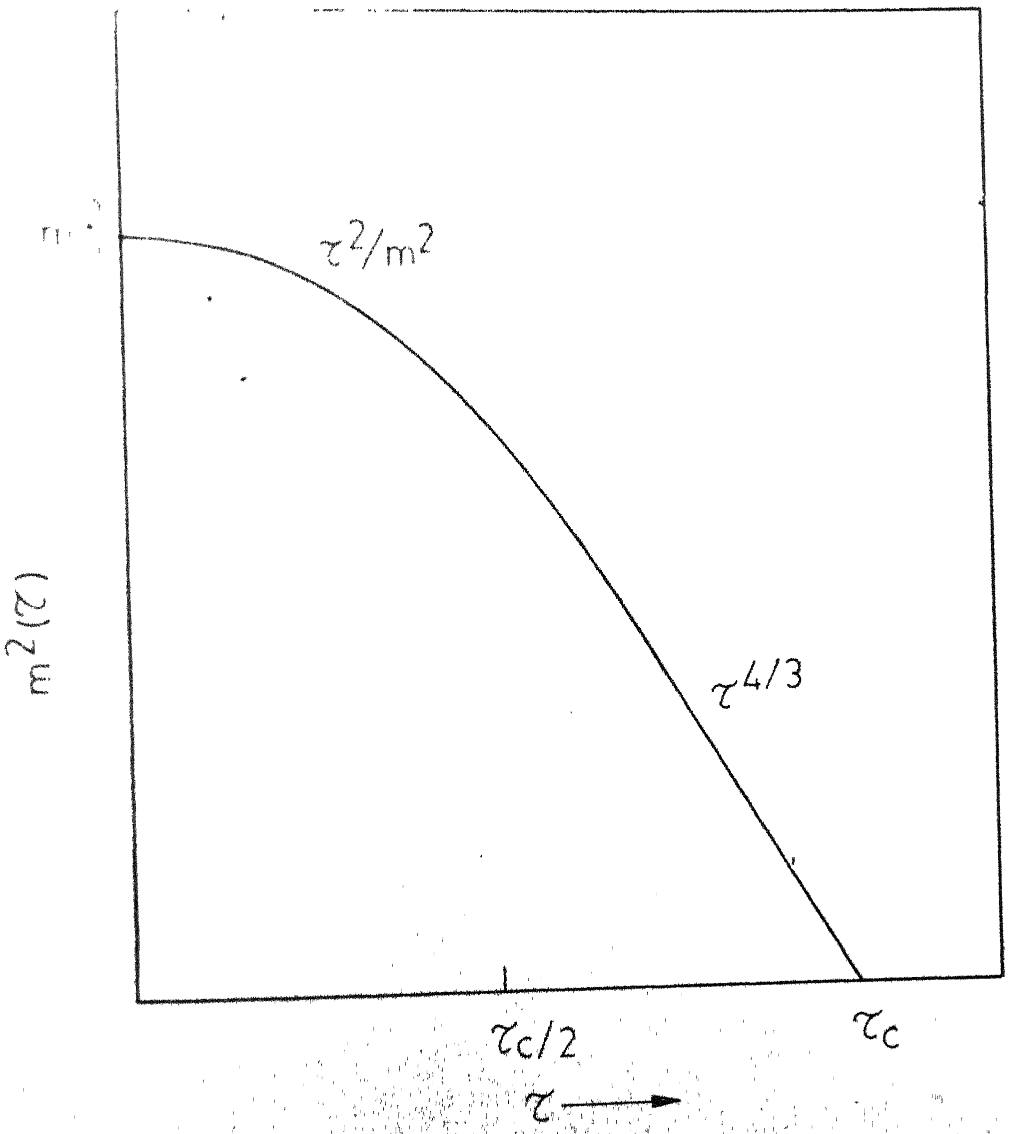


Fig. 18. m(T) for weak ferromagnets.

[illegible] T [illegible]. Notice that there is a reduction of [illegible] due to spin fluctuations. This point [illegible] emphasized by Moriya and Kawabata. [illegible] $^{-1}(T)$ against T is sketched in Fig. 18 [illegible], e.g., $ZrZn_2$, Ni_3Ga, NiPt etc. the [illegible] seen, as predicted from (4.11). Further, [illegible] flattening out described by (4.14).

5. Arrott Plots

In this section we discuss the field dependence of magnetization. This is conventionally represented by a plot of curves for $M^2(H,T)$ against $H/M(H,T)$, known as Arrott plots.[69] In the realm of molecular field theory it can be shown that these are straight lines at $T = T_c$:

$$\frac{\mu_B H}{k_B T_c} = \frac{1}{3}\left(\frac{M}{M_o}\right)^3 + \frac{1}{5}\left(\frac{M}{M_o}\right)^5 + \dots \qquad (5.1)$$

This has been seen to indicate the onset of ferromagnetism. However, recently Wohlfarth[26] and others have discussed $M(H,T)$ for Ni-Pt alloys. The Arrott plots came out to be straight lines over a wide range of temperatures and applied fields. There are deviations from linearity for high temperatures and low H/M. This behaviour (linearity) has been attributed to the correctness of Stoner theory for weak itinerant ferromagnets, while the deviation is associated with clustering effects.

[illegible] Wohlfarth's calculation and then [illegible] fluctuation effects can be included.

[illegible] for the difference between the free [illegible] magnetically ordered and disordered [illegible]

$$\Delta F = \frac{1}{2} A(T) M^2(H,T) + \frac{1}{4} B(T) M^4(H,T) - HM(H,T). \quad (5.2)$$

[illegible] be valid over the whole temperature [illegible] ferromagnets. Minimizing ΔF leads to the [illegible] equation for M:

$$(A(T) + B(T) M^2(H,T)) M(H,T) = H \quad (5.3)$$

giving

$$A(T) = - [2\chi(0,T)]^{-1}$$

and $B(T) = (2M^2(0,T)\chi(0,T))^{-1}$

where

$\chi(H,T) = [\partial M(H,T)/\partial H]_{H,T}$ is the high field susceptibility. Using the Stoner results

$$M^2(0,T) = M^2(0,0)\,[1-T^2/T_c^{\,2}]$$

and $\chi(0,T) = \chi(0,0)\,[1-T^2/T_c^{\,2}]^{-1}$

one gets

$$\left[\frac{M(H,T)}{M(0,0)}\right]^2 = 1 - (T/T_c)^2 + \frac{2\chi_o H}{M(H,T)} . \quad (5.4)$$

This is the Arrott plot expression extended to a wider temperature range. The slope of straight lines $H^2(H,T)$ against H/M is independent of temperature.

To consider the effect of spin fluctuations on (5.4), we include the magnetic field effects in the expression (2.3) for the partition function. This will add a term $\frac{g\mu_B}{c^z} H(=h)$ to the molecular field ξ_0. Therefore, the analysis of the section 2 can be applied directly, leading to

$$2\xi_0 - \beta c^z \left(\langle n_\uparrow \rangle_{\xi_0+h} - \langle n_\downarrow \rangle_{\xi_0+h}\right) = 0 \qquad 5.5$$

This is the equation for $\xi_0(h,T)$ (or $m(h,T)$). Including the effect of fluctuation self energy to the lowest order and carrying out the calculation similar to section 3 and 4, we find

$$m + (m+h)\left\{ - U\rho_{\epsilon_F}(T) + \frac{U_4}{U}\left(2D^T + 3D^L\right) + \right.$$
$$\left. + 2U_4 (m+h)^3 \right\} = 0 \qquad (5.6)$$

Retaining only term linear in h and using the expression (3.5) for m(0,T) we get

$$m(h,T)^2 - m(0,T)^2 = \frac{h(1+U_4 m^2(0,T))}{U_4\ m(h,T)} \qquad (5.7)$$

This expression will obviously give a different m(h,T). Now there is a temperature dependent factor introduced in h/m. At low temperatures this gives an expression similar to (5.4). At higher temperatures since $m^2(0,T)$

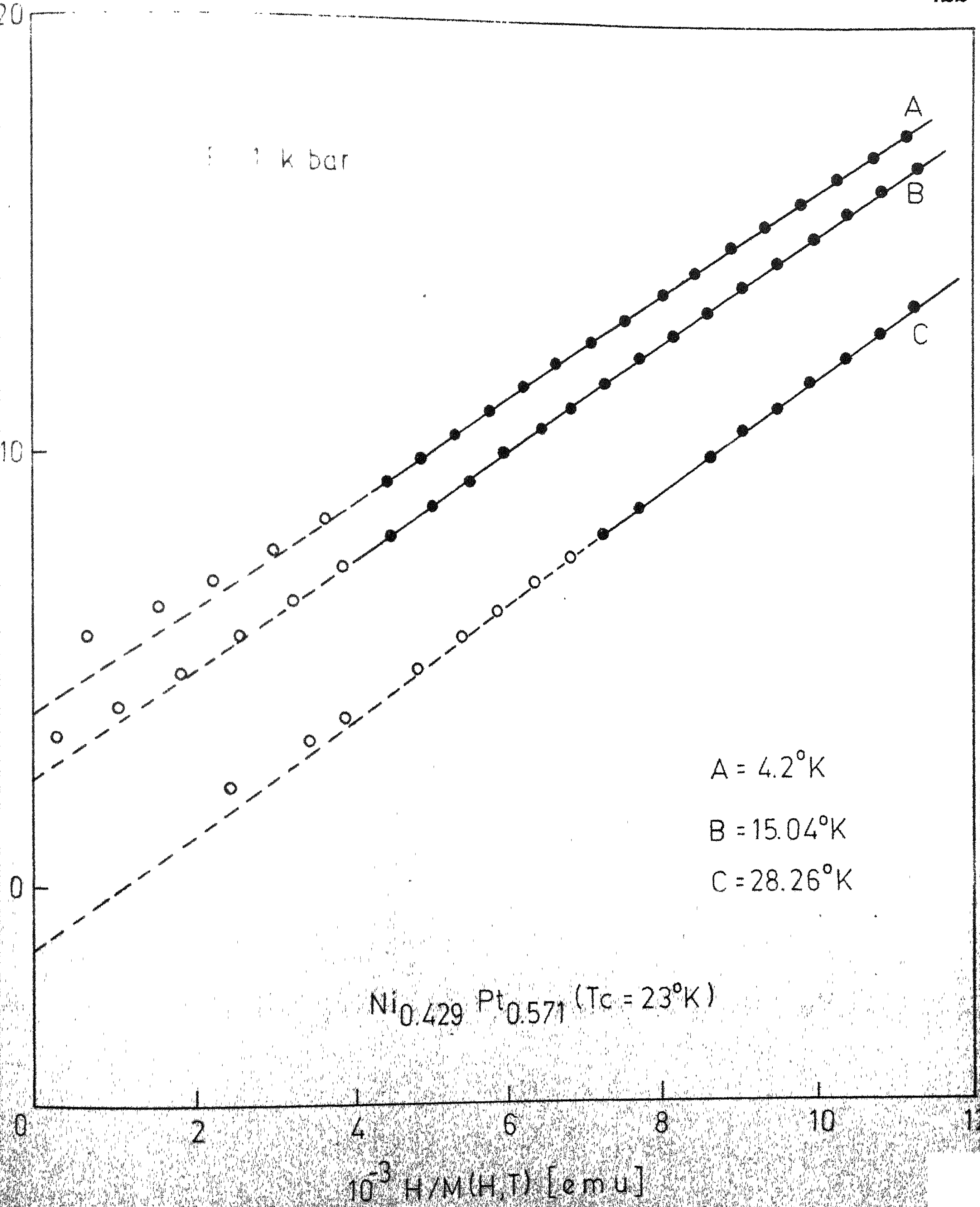


Fig. 19 - Arrott plot of M^2 vs. H/M for a Ni-Pt alloy.

varies as $T^{4/3}$, the parameters fixed for low temperature points will not give agreement in the high temperature regime, and hence the deviation. Since m^2 decreases with temperature, the slope $(m(H,T)^2 - m(0,T)^2)/(H/M(H,T))$ will decrease with increasing temperature, in agreement with the experiment (Fig. 19).

CHAPTER VI

SPIN WAVE STIFFNESS

1. Introduction

Spin waves exist as well defined, gapless, collective modes in isotropic ferromagnets. Their existence can be established in either of the models of ferromagnetism, i.e. Heisenberg model or an itinerant electron model. In fact, they are associated with the breaking of rotational symmetry at the second order phase transition point, T_c. The energy of this mode for small wave vector q is given by

$$\omega = Dq^2 \tag{1.1}$$

The coefficient D is known as spin wave stiffness. It is related to exchange integrals etc. As the temperature of the system is increased above 0°K, the energy of the mode keeps on decreasing. Above the transition point there are no long-wavelength spin waves. Since we have seen earlier that the temperature dependence of physical properties in weak ferromagnets is dominated by spin fluctuation effects, it is obviously relevant here to discuss D(T) and effects of spin fluctuations on it, in an itinerant electron model for weak ferromagnets.

We first discuss earlier theories, for orientation.

In the RPA,[6] the transverse spin susceptibility $\chi^{+-}(\vec{q},\omega)$ is calculated in the ladder approximation. It develops a pole when the zero range repulsive interaction U attains the value implied by the Stoner criterion $U\rho_{\varepsilon_F}=1$. For larger values of U there is an exchange splitting. With the electron propagators appropriate to this polarised state

$$G_{\underline{k}\pm} = (\nu_l - \varepsilon_k \pm \Delta/2)^{-1}, \tag{1.2}$$

the susceptibility becomes,

$$\chi_{\underline{q}}^{+-} = \frac{\chi^{o}(\vec{q},\omega,\Delta)}{1 - U\chi^{o}(\vec{q},\omega,\Delta)} \tag{1.3}$$

Here χ^{o} is the generalization of the Pauli susceptibility;

$$\chi^{o}(\vec{q},\omega,\Delta) = -\frac{1}{\beta}\sum_{\underline{k}} G_{\underline{k}\downarrow}\, G_{\underline{k}+\underline{q}\uparrow} .$$

The character of the singularity in $\chi(\vec{q},\omega)$ for small $|\vec{q}|$ and ω is then determined by the Goldstone theorem. Specifically, when the ground state spontaneously breaks the symmetry of the Hamiltonian via a non-zero Δ, that symmetry must be realized by a Goldstone boson, whose energy goes to zero in the limit of infinite wavelength. That is, a uniform rotation of all spins costs no energy. This implies that $\chi^{+-}(\vec{q},\omega)$ has a pole at zero $\vec{q}$ and ω. We have

$$1 = U\chi^o(0,0,\Delta) = \frac{U}{\Delta}\frac{1}{\beta}\sum_{\underline{k}}(G_{\underline{k}\uparrow} - G_{\underline{k}\downarrow}) = \frac{U}{\Delta}\, m,$$

where m is the magnetization. This equation determines Δ, which is just the Hartree-Fock exchange splitting. The Goldstone boson is a spin wave and we obtain its energy ω_q as a function of q by solving for the poles in $\chi(\vec{q},\omega)$

$$1 - U\chi^o(q,\omega,\Delta) = 0 \qquad (1.4)$$

For long wavelengths the result is

$$\omega(\vec{q}) = \frac{1}{m}\sum_{\vec{k}}\Big[\frac{1}{2}(n_{k\uparrow} + n_{k\downarrow})\left(q\cdot\frac{\partial}{\partial\vec{k}}\right)^2 \varepsilon_k - \frac{(n_{k\uparrow} - n_{k\downarrow})}{Um}\left(q\cdot\frac{\partial\varepsilon_k}{\partial k}\right)^2\Big] \qquad (1.5)$$

However, if the q value of the spin wave is large enough, greater than certain q_{max}, this pole will merge with the continuum, i.e. spin wave decays into an electron-hole pair and is a resonance in the magnetic response. The details of spectrum of these transverse excitations are shown in Fig. 20.

For a cubic lattice Eqn. (1.5) gives

$$D = \frac{U}{3}\sum_k\left\{\frac{n_{k\uparrow} + n_{k\downarrow}}{2\Delta}\nabla_k{}^2\varepsilon_k - \frac{n_{k\uparrow} - n_{k\downarrow}}{\Delta^2}(\nabla_k\varepsilon_k)^2\right\} \qquad (1.6)$$

Inserting in this equation the values of one electron energies, one can investigate the dependence of D on band structure, electron number, exchange splitting, magnetization etc. For weak ferromagnets ($m_o \ll 1$), by expanding D

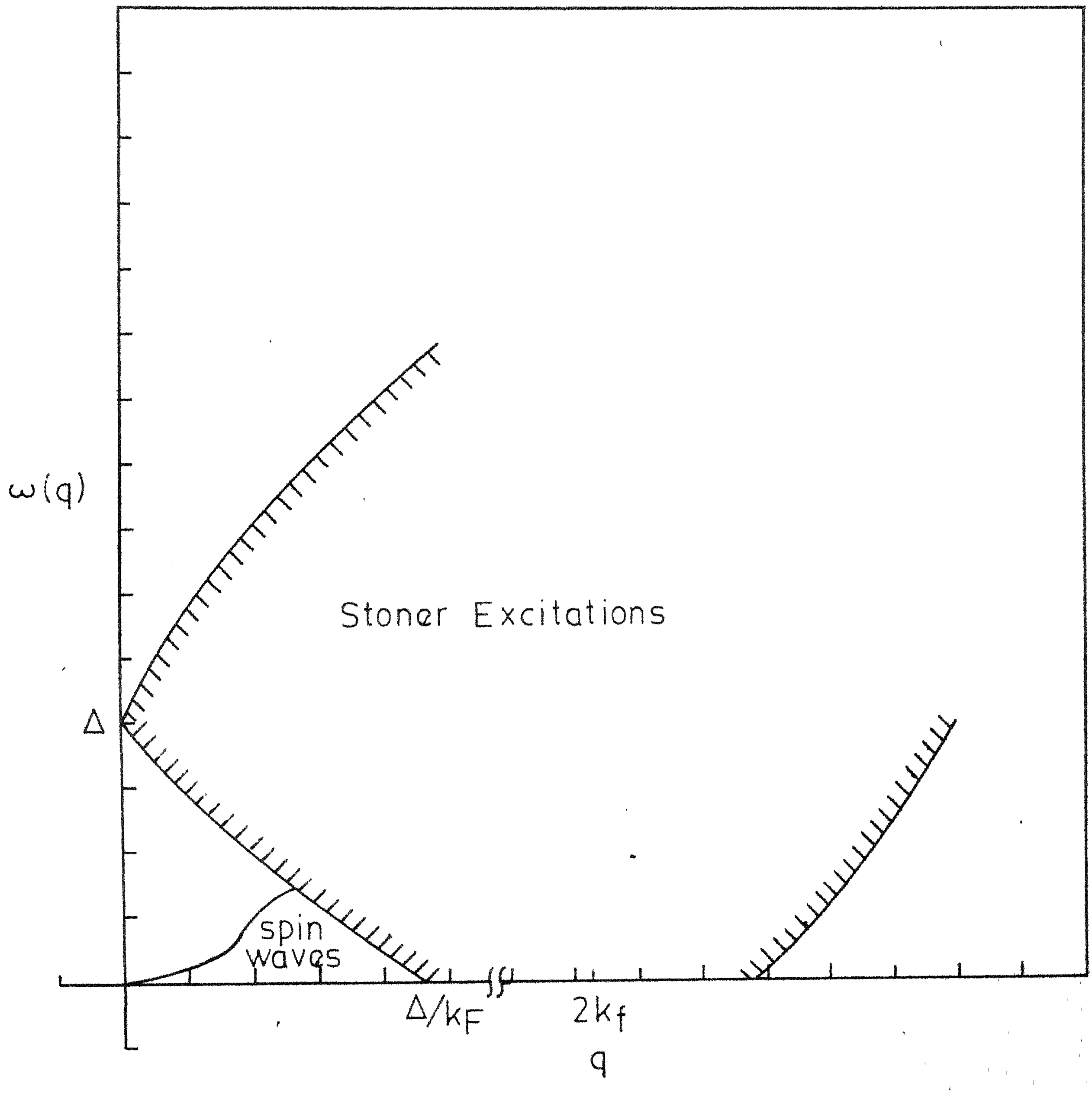


Fig. 20 - Electron - hole excitation spectrum (transverse) for an itinerant ferromagnet.

in powers of magnetization, a linear relation between D(T) and m(T) has been obtained.[70,71] This relation is analogous to the dependence deduced from the Heisenberg model for insulators. In general, D goes to zero simultaneously with the exchange splitting Δ at T_c. Using the same eqn. Mathon and Wohlfarth[72] have shown that

$$D = D_o + D_1 T^2, \tag{1.7}$$

and have calculated D_1 for tight binding bands. For this they have used the Stoner expression for m(T).

Recently Young[9] has improved the RPA expression for D taking into account the correlation effects in the T-matrix approximation. A T^2 term for D(T) has been isolated by using the Sommerfeld expansion of various temperature dependent functions (e.g. the single particle occupation number, the average t-matrix etc.). He has evaluated D_o and D_1 for a f.c.c. lattice with first and second neighbour interactions.

Thus in RPA the stiffness has basically a T^2 dependence because of the thermal single particle excitations, but the coefficient ($\sim \rho^2_{\varepsilon_F}$) is too small, by orders of magnitude, compared to what is observed in, say, Ni.

Izuyama and Kubo[27] have discussed the temperature dependence of D on general phenomenological considerations, as follows.

To lowest order the Hamiltonian of interacting spin waves can be written as

$$H = \sum_{\vec{k}} n_{\vec{k}} \Omega_k - \sum_{\vec{k}\vec{k}'} n_{\vec{k}} n_{\vec{k}'} C_{\vec{k}\vec{k}'} . \qquad (1.8)$$

n_k is the number of spin waves with energy Ω_k and $C_{kk'}$ is the quadratic coupling. In the mean field approximation one decouples the second term, getting

$$H = \sum_{\vec{k}} (\Omega_{\vec{k}} - 2 \sum_{\vec{k}'} C_{\vec{k}\vec{k}'} < n_{\vec{k}'} >) n_{\vec{k}} \equiv \sum_{\vec{k}} E_{\vec{k}} n_{\vec{k}} \qquad (1.9)$$

In the interaction term in $E_{\vec{k}}$ the only dependence on k arises from the coefficient $C_{kk'}$. C must go to zero as $k \to 0$, otherwise E_k would possess an energy gap at k=0. Because we expect $E_k \sim k^2$ at small k and since $C_{kk'}$ is symmetric in k and k', $C_{kk'} \sim \alpha k^2 k'^2$. On taking $\Omega = Dk^2$ one has

$$\begin{aligned} E_k &= k^2 \{D - 2\alpha \sum_{\vec{k}'} k'^2 < n_{\vec{k}'} >\} \\ &= k^2 \{ D - \alpha' (k_B T/D)^{5/2} \} \qquad (1.10) \end{aligned}$$

to first order in α . Thus spin wave interaction gives rise to a $T^{5/2}$ term in D(T). This dependence is the same as in Heisenberg model.[73] Obviously so, since the assumptions made are exactly valid for either model.

The effect of interaction between spin waves and the thermal electrons has been considered by writing the Hamiltonian as

$$H_{el,s.w} = \sum_{\vec{k}} n_{\vec{k}} \Omega_{\vec{k}} - \sum_{\vec{k}\vec{k}'} n_{\vec{k}} n_{\vec{k}'} C_{\vec{k}\vec{k}'}$$
$$+ \sum_{\vec{k}} \varepsilon_{\vec{k}} \delta n_{\vec{k}} - \sum_{kk'} \bar{C}_{\vec{k}k'} \delta n_{\vec{k}} \delta n_{\vec{k}'}$$
$$- \sum_{\vec{k}} C'_{\vec{k}\vec{k}'} n_{\vec{k}} \delta n_{k'} \quad . \tag{1.11}$$

δn_k is the number operator for the thermally excited electrons and C' is the electron-spin wave coupling. Again in the m.f.a.,

$$E_{\vec{k}} = \Omega_{\vec{k}} - 2 \sum_{\vec{k}'} C_{\vec{k}\vec{k}'} \langle n_{k'} \rangle - \sum_{\vec{k}'} C'_{\vec{k}\vec{k}'} \langle \delta n_{k'} \rangle \quad .$$

The last term will obviously give a T^2 contribution to $D(T)$. Hence

$$D(T) = D_0 - D_1 T^2 - D_2 T^{5/2} \quad . \tag{1.12}$$

The above qualitative prediction is supported by neutron diffraction results on Fe and Ni.[74,75] But there is an ambiguity about the exact power law obeyed by $D(T)$. For example, the spin wave resonance results[29] suggest; say, for Fe above 100°K, a $T^{3/2}$ dependence for $1 - D_T/D_0$. Similarly for Ni-Fe films the swr results agree with

$$D = D_0 \,(1 - a\, T^{5/2}) \text{ for } T < 80°K$$

and $D = D_1 \,(1 - a\, T^{3/2})$ for $T > 90°K$.

Moreover, the observed change with temperature is much larger than that predicted by theory. The conclusion is

that there is a need for investigation of $D(T)$ beyond mean field (RPA) theories.

The only interactions taken into account in RPA are the scattering of single electrons against the Fermi sea of electrons of opposite spin (the molecular field of this problem) and the resonant scattering of electron and hole of opposite spins responsible for the spin wave pole in χ. Interactions between the single particle excitations and the spin fluctuations are ignored. As elsewhere, these should have important effects here also. The problem is to incorporate these effects in a spin conserving manner. The standard way of doing this is via a Ward identity. Recently there has been progress in this direction due to Hertz and Edwards.[76] Using Ward identity they have discussed the effect of electron-magnon interaction on the structure of single particle self energy, spectral functions and spin wave stiffness constant at zero temperatures. We modify and apply their analysis to the problem at hand.

2. Formal Results a la Hertz-Edwards

The spin wave stiffness has a simple relation[76] with $\vec{\gamma}(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow)$, the irreducible part of the spin flip current vertex $\vec{\Gamma}(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow)$ for coupling to an external spin flip field:

$$m\,Dq^2 = C(\vec{q}) - q_\alpha \frac{1}{\beta} \sum_{\underline{k}} \gamma_\alpha(\underline{k}\downarrow, \underline{k}\uparrow)\, G_{\underline{k}\downarrow} G_{\underline{k}\uparrow} (\nabla_{\vec{k}}\, \varepsilon_{\vec{k}})_\beta\, q_\beta \tag{2.1}$$

where

$$C(\vec{q}) = \frac{1}{N} \sum_{\vec{k}} (\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}) \langle n_{\vec{k}\uparrow} - n_{\vec{k}+q\downarrow} \rangle$$

$$= \frac{1}{2N} q_i q_j \sum_k \frac{\partial^2 \varepsilon_k}{\partial k_i \, \partial k_j} \langle n_{k\uparrow} + n_{k\downarrow} \rangle \tag{2.2}$$

to order $|\vec{q}|^2$. Thus the knowledge of $\vec{\gamma}$ and the Green's function suffices to determine D. We have to calculate $\vec{\gamma}$ and G's in an approximation scheme. The scheme should be spin conserving so that the spin wave have correct dispersion at low momentum. Edwards and Hertz[76] show explicitly that the satisfaction of Ward identity implies that spin waves will have $\omega = Dq^2$ and not $\omega = A + Dq^2$. The Ward identity is a relation between the vertex Γ and the propagator G. An arbitrary approximation for G (i.e. the single particle self energy Σ) and an equally arbitrary approximation for Γ will not satisfy the Ward identity. There are standard prescriptions for choosing the vertex Γ given a G or Σ such that WI is satisfied. The choice of Σ is to be motivated physically.

The Ward identity as obtained by Hertz and Edwards is

$$q^\mu \Gamma_\mu (\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) \equiv q_0 \Gamma_0 (\underline{k}\uparrow, \underline{k}-\underline{q}\uparrow) - \vec{q} \cdot \vec{\Gamma} (\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow)$$

$$= G_\downarrow^{-1} (\underline{k}) - G_\uparrow^{-1} (\underline{k}-\underline{q}). \tag{2.3}$$

We analyze the equation (2.3) closely and try to get a simple criterion which follow as a consequence. We first

define the various terms involved. Γ_0 is the vertex for coupling to an external spin flip field. It is related to the transverse susceptibility by

$$\chi(\underline{q}) = \frac{1}{\beta} \sum_{\underline{k}} \Gamma_0 (\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) \; G_\downarrow(\underline{k}) \; G_\uparrow(\underline{k}-\underline{q}) \qquad (2.4)$$

Γ_0 is reducible. Consider $\gamma(\underline{k},\underline{k}-\underline{q})$, the irreducible part of Γ_0. Figure 21 shows the relation between Γ_0 and γ. If we divide any reducible diagram for Γ at its right most part of reducibility, everything to the left of that point is a contribution to full $\chi(q)$ and everything to the right a contribution to $\gamma(\underline{k}, \underline{k}-\underline{q})$:

$$\Gamma_0 (\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) = \gamma(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) + U\,\chi(q)\,\gamma(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) \quad (2.5)$$

A similar analysis can be applied to the diagrammatic structure of the perturbation series for $\vec{\Gamma}$, giving

$$\vec{\Gamma}(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) = \vec{\gamma}(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) + U\,\vec{\chi}_{JS}(q)\,\gamma(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) \quad (2.6)$$

where $\vec{\gamma}$ is the irreducible part of $\vec{\Gamma}$ and $\vec{\chi}_{JS}$ is the spin density current susceptibility:

$$\vec{\chi}_{JS} = \langle T\,(\vec{J}^{\,+}_{\vec{q}}(u)\; S^-_{-\vec{q}}(u'))\rangle$$

which satisfies

$$\vec{\chi}_{JS}(\underline{q}) = \frac{1}{\beta} \sum_{\underline{k}} \vec{\Gamma}(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow)\; G_{\underline{k}\downarrow}\; G_{\underline{k}\;q\uparrow}\,.$$

We need one more relation, between $\vec{\chi}_{JS}$ and χ, which from

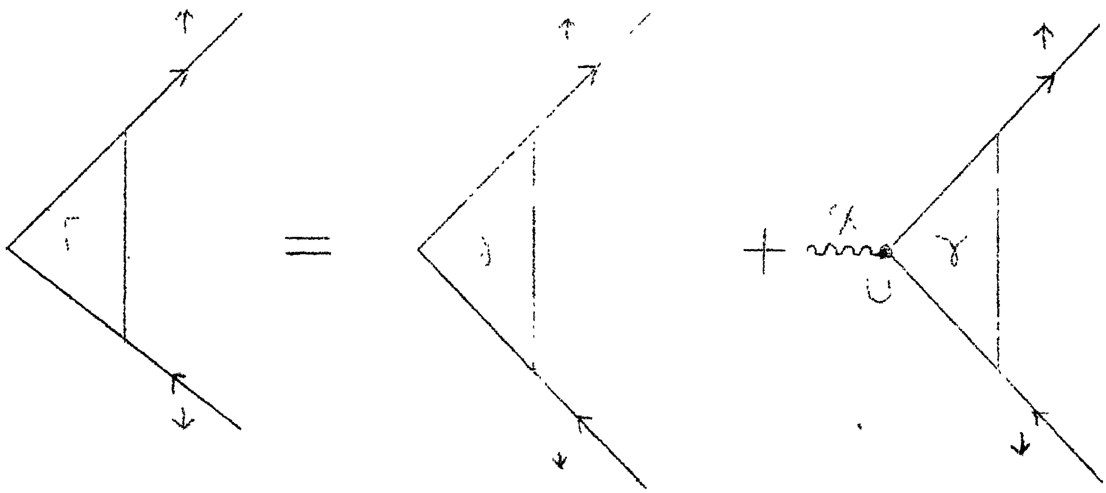


Fig. 21. The structure of the reducible vertex Γ.

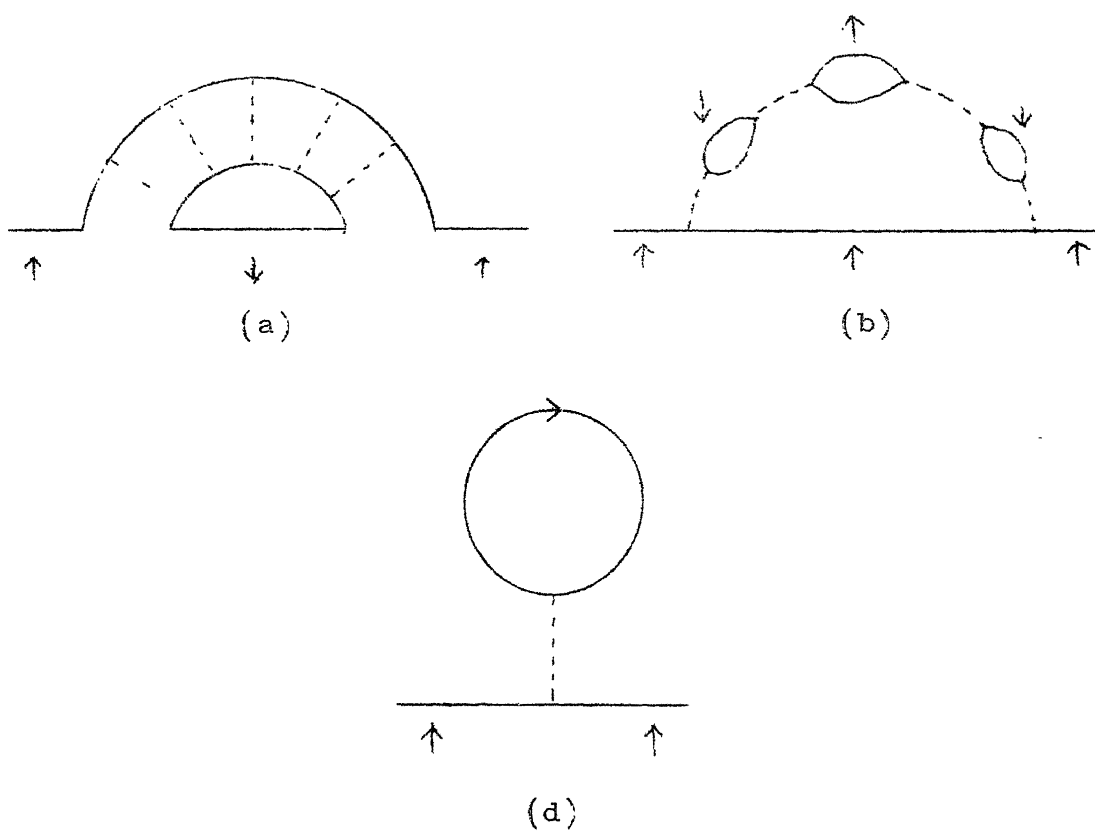


Fig. 22. The lowest order class of self energy corrections due to (a) transverse fluctuations (Ladder series) (b) longitudinal fluctuations (Ring series) (c) Hartree term.

the equation of motion of $\chi(\vec{q}, u-u')$, is

$$\vec{q} \cdot \vec{\chi}_{JS}(\underline{q}) = q_o \, \chi(\underline{q}) + m \tag{2.7}$$

Combining equations (2.5), (2.6) and (2.7) with (2.3), we find

$$G^{-1}_{\underline{k}\downarrow} - G^{-1}_{\underline{k}-\underline{q}\downarrow} = (q_o - \Delta) \; \gamma(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow) - \vec{q} \cdot \vec{\gamma}(\underline{k}\downarrow, \underline{k}-\underline{q}\uparrow),$$

which at $\vec{q}=0$, $q_o(\equiv\omega) = 0$ reads

$$\gamma(\underline{k}\downarrow, \underline{k}\uparrow) = 1 - (\Sigma_{\underline{k}\uparrow} - \Sigma_{\underline{k}\downarrow})/\Delta \tag{2.8}$$

Here we have used

$$G^{-1}_{\sigma} = G^{o-1}_{\sigma} - \Sigma_{\sigma} .$$

The equation (2.8) gives a relation between Σ and the scalar γ obeying the Ward identity. Once we get diagrams for γ corresponding to an approximation for Σ we can construct diagrams for the vector vertex $\vec{\gamma}$ and hence calculate $D(T)$. We use the equation (2.8) to check explicitly whether our approximation scheme satisfies the Ward identity.

3. The Self Energy and Scalar Vertex

We have first to choose an electron self energy function Σ. Since the vertex is obtained by differentiation of particle or hole lines in diagrams for Σ; one

necessarily requires an explicit diagrammatic form for Σ. This somewhat limits the (temperature) range of our results, since the self consistency present in our earlier results (for $\chi(T)$, M^2 etc.) will no longer be true. We shall obtain results for $\mathbf{D}$ in an approximation where the leading fluctuation effects at low temperatures are correctly included.

So far we have been working with the Hamiltonian involving electrons plus interacting fluctuation fields. Since we have to work with electronic degrees of freedom explicitly in order to formulate Σ, γ etc., the logical thing to do is to integrate out the fluctuation field to get back the interacting electron system. This gives

$$H = T + V , \quad \text{where } V = -\frac{2}{3}U\,\vec{S}.\vec{S} .$$

Except for a one body term, the potential energy can be reexpressed in terms of the well known Hubbard model,

$$H = T + U\, n_{i\uparrow}\, n_{i\downarrow} . \tag{3.1}$$

The spin fluctuation effects are contained in the propagators D^T and D^L (or χ^{+-} and χ^{zz}). For a weak ferromagnet, the former has a low lying resonance (energy $m^2\ \varepsilon_F$) while the latter has a spin wave pole, again low-lying because of small stiffness. We therefore use for Σ an approximation where the electron couples to χ^{zz} and χ^{+-}.

waves with $\omega = Dq^2$ as already discussed.

Next considering the diagrams Fig. 22a and b, we find

$$\Sigma_{\underline{k}\uparrow} = \frac{1}{\beta} \sum_{\underline{q}} U^2 (\chi^{+-}_{\underline{q}} \, G_{\underline{k}-\underline{q}\downarrow} + \chi^{-}_{\underline{q}} \, G_{\underline{k}-\underline{q}\uparrow}) + U \langle n\downarrow \rangle \qquad (3.3a)$$

and

$$\Sigma_{\underline{k}\downarrow} = \frac{1}{\beta} \sum_{q} U^2 \, (\chi^{-+}_{\underline{q}} \, G_{\underline{k}-\underline{q}\uparrow} + \chi^{+}_{\underline{q}} \, G_{\underline{k}-\underline{q}\downarrow}) + U \langle n\uparrow \rangle \qquad (3.3b)$$

where

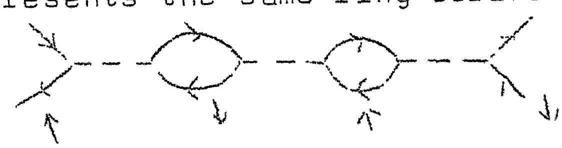
$$\chi^{+-}_{\underline{q}} = \frac{\chi^{o+-}_{\underline{q}}}{1 - U \chi^{o+-}_{\underline{q}}} ,$$

$$\chi^{\pm}_{\underline{q}} = \frac{\chi^{o\pm}_{\underline{q}}}{1 - U^2 \chi^{o+}_{\underline{q}} \chi^{o-}_{\underline{q}}} ,$$

$$\chi^{o+-}(\underline{q}) = -\frac{1}{\beta} \sum_{\underline{k}} G_{\underline{k}\downarrow} \, G_{\underline{k}+\underline{q}\uparrow}$$

and $\chi^{o\pm}(\underline{q}) = -\frac{1}{\beta} \sum_{k} G_{\underline{k}\sigma} \, G_{\underline{k}+\underline{q}\sigma}$.

The vertex γ is now obtained by inserting h^+ (wherever permissible) once in an internal bare line in the diagrams for the self energies we have just calculated. We get a set of diagrams represented in Fig. 23 b–f, where the hatched boxes represent one of the terms of the RPA ring (L) or the ladder (T) series and in f the double wavy line represents the same ring series with the first term being

 .

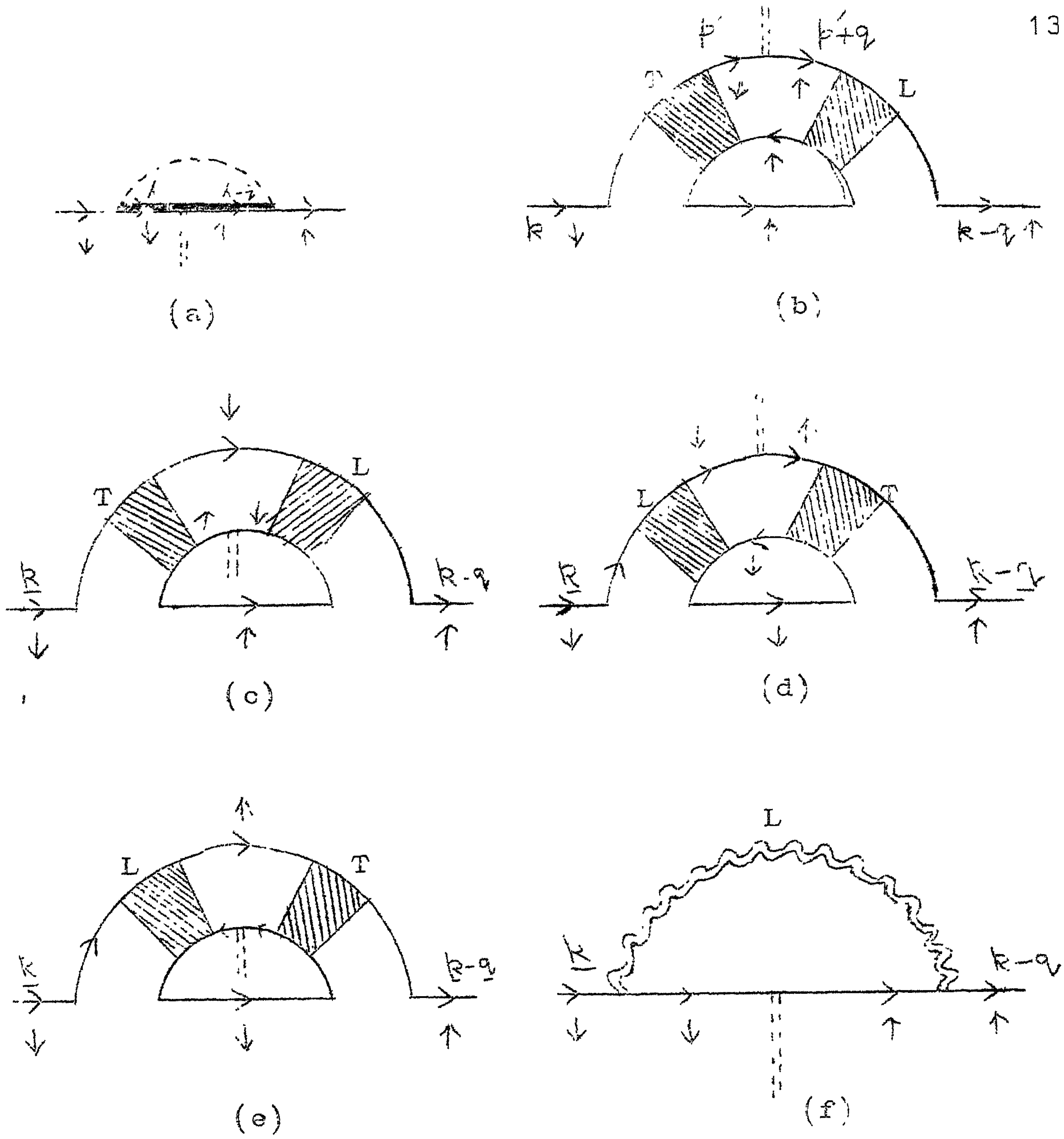


Fig. 23. The lowest order self energy diagrams with h^+ (====) inserted.

These diagrams represent the following expression for $\gamma(\underline{k}\downarrow,\ \underline{k}-\underline{q}\uparrow)$

$$\text{b:}\quad \frac{1}{\beta^2}\sum_{\underline{k}'\underline{q}'} G_{\underline{k}'\downarrow}\, G_{\underline{k}'-\underline{q}\uparrow}\, G_{\underline{k}+\underline{q}'\uparrow} \left(\frac{-U^3\ \chi^{-}_{-\underline{q}-\underline{q}'}}{1 - U\ \chi^{0+-}_{\underline{q}'}}\right) G_{\underline{k}'+\underline{q}'\uparrow}$$

$$\text{c:}\quad \frac{1}{\beta^2}\sum_{\underline{k}'\underline{q}'} G_{\underline{k}'\downarrow}\, G_{\underline{k}'-\underline{q}\uparrow}\, G_{\underline{k}+\underline{q}'\uparrow}\, G_{\underline{k}'-\underline{q}-\underline{q}'\downarrow}\ \frac{U^2}{(1 - U\ \chi^{0+-}_{\underline{q}'})(1 - U^2\ \chi^{0+}_{-\underline{q}-\underline{q}'}\,\chi^{0-}_{-\underline{q}-\underline{q}'})}$$

$$\text{d:}\quad \frac{1}{\beta^2}\sum_{\underline{k}'\underline{q}'} G_{\underline{k}'\downarrow}\, G_{\underline{k}'-\underline{q}\uparrow}\, G_{\underline{k}+\underline{q}'\downarrow}\, G_{\underline{k}'+\underline{q}'\downarrow}\ \frac{-U^3\ \chi^{+}_{\underline{q}'}}{(1 - U\ \chi^{0+-}_{-\underline{q}-\underline{q}'})}$$

$$\text{e:}\quad \frac{1}{\beta^2}\sum_{\underline{k}'\underline{q}'} G_{\underline{k}'\downarrow}\, G_{\underline{k}'-\underline{q}\uparrow}\, G_{\underline{k}+\underline{q}'\uparrow}\, G_{\underline{k}-\underline{q}-\underline{q}'\uparrow}\ \frac{U^2}{(1 - U\ \chi^{0+-}_{-\underline{q}-\underline{q}'})(1 - U^2\ \chi^{0+}_{\underline{q}'}\ \chi^{0-}_{\underline{q}'})}$$

$$\text{f:}\quad \frac{1}{\beta}\sum_{\underline{q}'} G_{\underline{k}-\underline{q}'\downarrow}\, G_{\underline{k}-\underline{q}-\underline{q}'\uparrow}\ \frac{-U^3\ \chi^{0+}_{\underline{q}'}\ \chi^{0-}_{\underline{q}'}}{(1 - U^2\ \chi^{0+}_{\underline{q}'}\ \chi^{0-}_{\underline{q}'})}\ .$$

We now check whether above set of diagrams for Σ and γ satisfy Eqn. (2.8). This can be done after some simplification and some algebra. The algebra is straightforward, the main simplification is in writing the product of three Green's functions as the difference between the free particle like susceptibilities. For example, consider

$$\frac{1}{\beta} \sum_{\underline{k}'} G_{\underline{k}'-\underline{q}\uparrow} G_{\underline{k}'\downarrow} G_{\underline{k}'+\underline{q}'\uparrow}$$

which for $\underline{q} = 0$, reduces to

$$\frac{1}{\beta} \sum_{k'} \frac{G_{\underline{k}'\downarrow} \; G_{\underline{k}'\uparrow}}{U_m + \Sigma_{k'\downarrow} - \Sigma_{k'\uparrow}} G_{\underline{k}' +\underline{q}'\uparrow}$$

$$\simeq \frac{1}{\beta} \sum_{\underline{k}'} \frac{(G_{\underline{k}'\downarrow} - G_{k'\uparrow})}{U_m} G_{\underline{k}'+\underline{q}'\uparrow}$$

$$= \frac{1}{U_m} (\chi^{0-+}_{\underline{q}'} - \chi^{0+-}_{\underline{q}'}).$$

This is correct to the lowest order in $\Sigma_{k'\sigma}$, which is what we consider. After such simplifications, adding all the diagrams for γ and Σ separately we easily get the desired result

$$\gamma(\underline{k}\downarrow, \underline{k}\uparrow) = 1 - \frac{\Sigma_{\underline{k}\uparrow} - \Sigma_{\underline{k}\downarrow}}{\Delta}$$

This confirms the correctness of our diagrammatic expression for γ starting from the approximation we have made for Σ_σ.

4. The Vector Vertex and D(T)

We consider a set of diagrams for $\vec{\gamma}$ exactly similar to that for γ. These diagrams can be classified physically into three categories; namely, the self energy correction to the RPA propagators, magnon drag and the vertex correction terms. In RPA, γ was unity and the

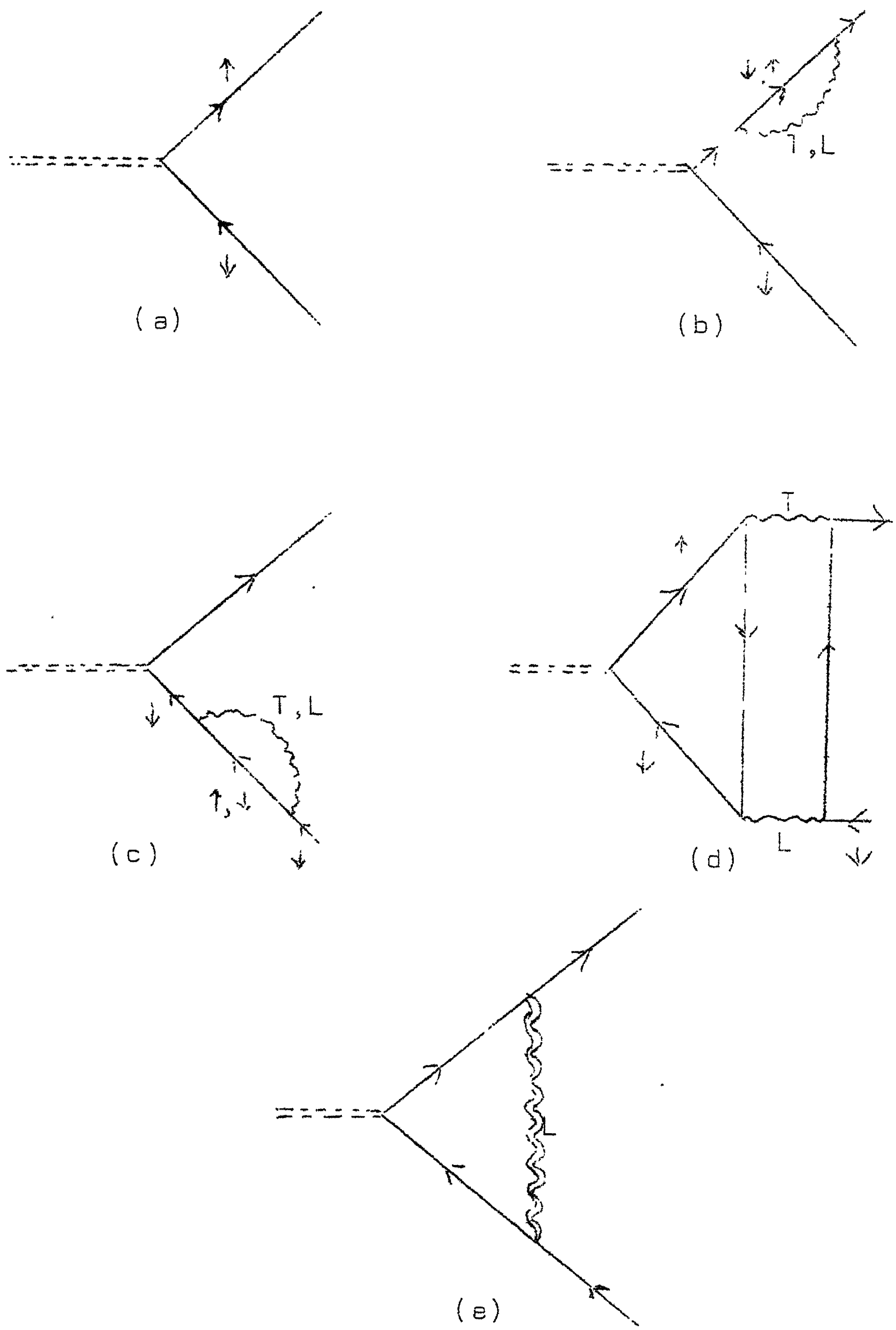


Fig. 24. Diagrams for the irreducible spin flip current vertex, $\vec{\gamma}$

(a) 'bare' RPA (b),(c) Self energy corrections

(d) Magnon 'drag' term (e) Vertex corrections.

propagators used were in HFA. In the first category the lowest order spin fluctuation self energy corrections are included (Fig. 24b,c). The magnon drag term is represented by diagrams b-e in Fig. 23. Physically, these diagrams represent inclusion of effect of fluctuation interaction or the 'magnon drag'. These diagrams are similar to two spin fluctuation diagrams considered earlier. These are also included in the phenomenological theory of Izuyama and Kubo. A typical diagram may be represented by Fig. 24d. The next set represents vertex or electron-hole wave function modification by longitudinal spin fluctuations (Fig.24e).

Now we consider the Hertz-Edwards equation (Eqn. 2.1) for stiffness. In RPA, for weak ferromagnets, the stiffness is proportional to magnetization. Here also, we expect similar results to hold except the fluctuation corrections. That is

$$m\,Dq^2 = A(T)\ m^2\ q^2 \tag{4.1}$$

to lowest order in m. This can be proved as follows: Consider relations

$$mDq^2 = C(\vec{q}) - \vec{q}\,.\,[\lim_{\omega\to 0}\ \lim_{|\vec{q}|\to 0}\ \overleftrightarrow{\chi}_{JJ}\ (\vec{q},\omega)]\,.\,\vec{q} \tag{4.2}$$

and

$$\omega[\omega\,\chi(\vec{q},\omega) + m] = -\,C(\vec{q}) + \vec{q}\,.\,\overleftrightarrow{\chi}_{JJ}(\vec{q},\omega)\,.\,\vec{q} \tag{4.3}$$

from HE. Since $\lim_{\omega\to 0} \lim_{|\vec{q}|\to 0} \chi(\vec{q},\omega) \sim \frac{q^2}{\omega}$,

$$[mD]_{m\to 0} = \frac{C(q)}{q^2} - \lim_{\omega\to 0} \lim_{|\vec{q}|\to 0} \lim_{m\to 0} \chi_{JJ}(\vec{q},\omega)$$

$$= \frac{C(q)}{q^2} - \frac{C(q)}{q^2} - \left(\frac{\omega^2 - q^2}{\omega}\right) \begin{array}{l}\lim |\vec{q}|\to 0\\ \lim \omega\to 0\end{array}$$

$$= 0$$

Thus mDq^2 does not have any term independent of m. The lowest order term should be of order m^2. Therefore we expand each term on RHS of Eqn. (2.1) and examine the thermal contribution to the coefficient of m^2 term.

We now analyze D(T) considering various contributions to γ_α.

<u>a. Bare RPA</u> : This corresponds to $\gamma = 1$ and hence $\gamma_\alpha = k_\alpha$. The propagators $G_{\underline{k}\sigma}$ are the Hartree Fock one,

$$G^o_{\underline{k}\sigma} = (\nu_1 - \varepsilon_{\vec{k}} + \sigma\frac{\Delta}{2})^{-1}.$$

This gives

$$q \cdot \frac{1}{\beta} \sum_{\underline{k}} \vec{\gamma}(\underline{k}\downarrow, \underline{k}\uparrow)\, G^o_{\underline{k}\uparrow} G^o_{\underline{k}\downarrow} \vec{\nabla}_{\vec{k}}\, \varepsilon_{\vec{k}} \cdot \vec{q}$$

$$= q_\alpha\, q_\beta \frac{1}{\beta} \sum_{\underline{k}} k_\alpha\, k_\beta \left\{ \frac{1}{\nu_1 - \varepsilon_{\vec{k}} + \Delta/2} \quad \frac{1}{\nu_1 - \varepsilon_{\vec{k}} - \Delta/2} \right\}$$

Expanding in powers of Δ, the lowest term is of order Δ^2, we find

$$m(T)\ D_1\ (RPA) = \frac{\varepsilon_f\ \rho''_{\varepsilon_F} + 2\rho'_F}{36}\ \Delta^2\ . \qquad (4.4)$$

This is the well known result for low magnetization.

b. Self energy corrections : Here we dress the HF propagators with the transverse and longitudinal fluctuation lines. This is represented in Fig. 24 b & c and contributes

$$q_\alpha q_\beta \frac{1}{\beta} \sum_{\underline{k}} k_\alpha k_\beta\ G^o_{\underline{k}\uparrow}\ G^o_{\underline{k}\downarrow}\ [\Sigma_{\underline{k}\uparrow}\ G^o_{\underline{k}\uparrow} + \Sigma_{\underline{k}\downarrow}\ G^o_{\underline{k}\downarrow}]$$

to lowest order in Σ. We have already discussed the approximation scheme for Σ's. Substituting those expressions, we find to order Δ^2

$$q_\alpha q_\beta\ \Delta^2 \{\frac{1}{\beta} \sum_{\underline{k}} k_\alpha k_\beta\ G^{o\ 6}_{\underline{k}}\}\ \{\frac{U^2}{\beta}\sum_{\underline{q}} \chi^{+-}(\underline{q}) + \chi^+(\underline{q}) + \chi^-(\underline{q})\}$$

$$+ q_\alpha q_\beta\ \Delta\{\frac{1}{\beta} \sum_{\underline{k}} k_\alpha k_\beta\ G^{o5}_{\underline{k}}\}\ \{\frac{U^2}{\beta} \sum_{\underline{q}} (\chi^+(\underline{q}) - \chi^-(\underline{q})\}$$
(4.5)

The integrals will give a $m(T)\ (T/D)^{3/2}$ contribution from $\chi^{+-}(\underline{q})$ (due to spin wave pole) and a T^2/m^2 term from the longitudinal fluctuations. This has already been discussed in detail in Chapter V.

c. Vertex correction : This is given in Fig. 24 f and contributes

$$\vec{q}\ .\ \frac{1}{\beta^2} \sum_{\underline{k},\underline{q}'} G_{\underline{k}\uparrow}\ G_{\underline{k}\downarrow}\ (\vec{k}+\vec{q}')\ G_{\underline{k}+\underline{q}'\uparrow} G_{\underline{k}+\underline{q}'\downarrow}$$

$$\times\ \{\frac{U^3\ \chi^{o+}_{\underline{q}'}\ \chi^{o-}_{\underline{q}'}}{1 - U^2\ \chi^{o+}_{\underline{q}'}\ \chi^{o-}_{\underline{q}'}}\}\ \vec{\nabla}_{\vec{k}}\ \varepsilon_{\vec{k}}\ .\ \vec{q}\ .$$

We assume $\underline{q}'=0$ in comparison to the electron momentum energy $\underline{k}$ wherever possible so that the integration can be divided into two parts one involving sum over the product of four fermion propagators and the other involving sum over fluctuation term. The first part then again can be expanded in powers of Δ^2 giving

$$(mDq^2)_{vertex} = -\frac{1}{3}\Delta^2 q^2 \frac{1}{5!}(\varepsilon_f \; \rho''_{\varepsilon_F} + 4\rho'''_F)$$

$$\times \quad [(\frac{1}{\beta}\sum_{\underline{q}'} \frac{U^3 \; \chi^{o+}_{\underline{q}} \; \chi^{o-}_{\underline{q}}}{1 - U^2 \; \chi^{o+}_{\underline{q}'} \; \chi^{o-}_{\underline{q}'}})] \tag{4.6}$$

The integration over the longitudinal fluctuation propagator gives a τ^2/m^2 contribution.

d. The magnon drag term : This represents the effect of fluctuation interaction on the RPA term. There are four diagrams corresponding to this term (Fig.23b,c,d and e).

$$(\gamma_\alpha)^{MD}_b = -\frac{1}{\beta^2}\sum_{\underline{k}',\underline{q}'} k'_\alpha \quad G_{\underline{k}'\downarrow} \; G_{\underline{k}'\uparrow} \; G_{\underline{k}'+\underline{q}'\uparrow} \; G_{\underline{k}+\underline{q}'\uparrow} \; \frac{U^3 \; \chi^-_{-\underline{q}'}}{1 - U\;\chi^{o+-}_{\underline{q}'}}$$

$$(\gamma_\alpha)^{MD}_c = +\frac{1}{\beta^2}\sum_{\underline{k}'\underline{q}'} k'_\alpha \quad G_{\underline{k}'\downarrow} \; G_{\underline{k}'\uparrow} \; G_{\underline{k}'-\underline{q}'\downarrow} \; G_{\underline{k}+\underline{q}'\uparrow} \; \frac{U^2}{(1 - U^2 \; \chi^{o+}_{-\underline{q}'} \; \chi^{o-}_{-\underline{q}'})(1 - U\;\chi^{o+-}_{\underline{q}'})}$$

$$(\gamma_\alpha)_D^{MD} = -\frac{1}{\beta^2}\sum_{\underline{k}'\underline{q}'} k'_\alpha \; G_{\underline{k}'\downarrow}\, G_{\underline{k}'\uparrow}\, G_{\underline{k}'+\underline{q}'\downarrow}\, G_{\underline{k}+\underline{q}'\uparrow} \; \frac{U^3 \chi^{+}_{\underline{q}'}}{1 - U\chi^{0+-}_{-\underline{q}'}}$$

$$(\gamma_\alpha)_E^{MD} = +\frac{1}{\beta^2}\sum_{\underline{k}'\underline{q}'} k'_\alpha \; G_{\underline{k}'\downarrow}\, G_{\underline{k}'\uparrow}\, G_{\underline{k}'-\underline{q}'\uparrow}\, G_{\underline{k}+\underline{q}'\downarrow} \; \frac{U^2}{(1 - U^2\chi^{+}_{\underline{q}'}\chi^{-}_{\underline{q}'})(1 - U\chi^{0+-}_{-\underline{q}'})}$$

We substitute these into eqn. (2.1). As usual consider $\underline{q}'=0$ in the electron propagators. We will then have terms of the form

$$-\sum q_\alpha k'_\alpha \;(A_{k'} + \Delta B_{k'} + \Delta^2 C_{k'}) \times (A_k + \Delta B_k + \Delta^2 C_k)\; q_\beta k_\beta$$

$$\frac{1}{\beta}\sum_{\underline{q}'} \frac{U^3 \chi^{-}_{-\underline{q}'}}{(\text{-----})(\text{----})} \; .$$

$$= \sum_{\vec{k}'} (\vec{q}.\vec{k}')\, f_{k'} \sum_{\vec{k}} (\vec{q}.\vec{k})\, f_k \,\frac{1}{\beta}\sum_{\underline{q}'} \Gamma^L(-\underline{q}')\;\Gamma^T(\underline{q}')$$

We notice that on $\vec{k}$ or $\vec{k}'$ summation it will vanish, since $\sum_{\vec{k}}(\vec{q}\;.\;\vec{k})\;\phi_{\vec{k}}$ (scalar) = 0. Here we have defined

$$\frac{1}{\beta}\sum_{\nu_1} G_{\underline{k}'\downarrow}\, G_{\underline{k}'\uparrow}\, G_{\underline{k}'\uparrow} \cong (A_{\vec{k}'} + \Delta B_{\vec{k}'} + \Delta^2 C_{\vec{k}'}).$$

So nothing interesting survives if we put $\underline{q}'=0$. Now let us consider the full expression. This will involve the factors of the form

$$\frac{1}{\beta} \sum_{\underline{k}'} G_{\underline{k}'\downarrow} G_{\underline{k}'\downarrow} G_{\underline{k}'+\underline{q}'\uparrow} (\vec{q}.\vec{k}').$$

To the lowest order in $(\vec{q}.\vec{q}')$ the term can be written as

$$(A_1 + \Delta B_1 + \Delta^2 C_1)\ (\vec{q}.\vec{q}') + O(|\vec{q}.\vec{q}'|^2).$$

We proceed as before and find (after collecting a, b, c, d & e, terms and analyzing) that the surviving term is

$$(mDq^2)^{MD} \cong -\frac{q_\alpha q_\beta}{3} \Delta^2 \left(\frac{1}{\beta} \sum_{\underline{q}'} q'_\alpha\ q_\beta \Gamma^T_{\underline{q}'}\ \Gamma^L_{-\underline{q}'}\right). \qquad (4.7)$$

The most dominant term will be that from the pole of Γ^T and will contribute a $m(T)\ T^{5/2}$ term at low temperatures and hence negligible companion to T^2 etc. terms.

Collecting all the thermal contributions we can write the expression for D(T) as

$$D(T) = M(T)\left[m^{-1}\ D^{RPA} - A\frac{\tau^2}{m^2} - B\ m\ (\frac{\tau}{m})^{3/2} - C\ m\ (\tau/m)^{5/2}\right]. \qquad (4.8)$$

The coefficients A, B and C are given in terms of single particle density of states and its derivatives at fermi energy. Notice that at low temperatures there is a strong T^2 dependence, while at high temperatures D(T) is expected to decrease as $\tau m(T)$.

5. Discussion

The main qualitative features of our results Eq. (4.8) for D are: 1) an enhanced τ^2 dependence (enhanced doubly in powers of m^{-1}, a large quantity), 2) A reduced $\tau^{3/2}$ dependence (reduced by one power of m). The presence of a $\tau^{3/2}$ conflicts with the phenomenological result of Izuyama and Kubo who find only a $\tau^{5/2}$ term. It also conflicts with the result of Corrias and de Pasquale[28] who calculate (for a strong ferromagnet $\langle n_\uparrow \rangle = N$, $\langle n_\downarrow \rangle = 0$) the spin wave spin wave vertex $C(k,k')$ (see Eq. (1.9)) using a Ward like identity and show it to be of the form $k^2k'^2$ for small k,k'. (Both these authors find a τ^2 term.) We have no good explanation for this discrepancy. The $T^{3/2}$ term arises from a self energy correction to the single particle propagator in the particle hole term $G_{\underline{k}\uparrow}G_{\underline{k}\downarrow}$. We have looked for and not found any cancellation of this term to leading order in T. We are unable to cast our result in the Izuyama-Kubo form of i.e., we do not write the total energy of the system as a functional of the number of spin waves and of electrons. It is not clear that this can be done.

CHAPTER VII

CONCLUSION

In this chapter we make a few concluding remarks. We briefly summarize our approach and results, point out a few areas where more work needs to be done, and briefly discuss other phase transitions in fermi systems where fluctuation effects of the type considered might be relevant.

In this thesis, nearly and weakly ferromagnetic fermi systems have been considered. It is found that the thermal or temperature dependent properties are dominated by spin fluctuations and their interaction. Spin fluctuation excitations are of low energy, and are fairly stiff (their energy increases only slowly with increasing fluctuation wavevector q). They couple strongly amongst themselves and the coupling is basically of short range ($\sim k_F^{-1}$). The characteristic temperature dependences arising in physical properties as a result of coupling between these spin fluctuations can be explicitly determined in two extreme physical regimes i.e. the quantum or low temperature regime and the classical regime. Expressions retaining the leading temperature dependent

terms can be written down which cover these extremes and the intermediate region as well. Because the systems is by assumption at temperatures far below the free fermi temperature T_F^o, effects due to more than two correlated spin fluctuations are shown to be small. Since the two correlated spin fluctuation term behaves very much like the one spin fluctuation term, a simple Hartree like approximation (self consistent mean fluctuation field theory) is adequate generally. These considerations break down near the critical point. This critical regime shrinks exponentially as $T_c \rightarrow 0$. Because of the intermediate coupling nature of the problem, while the temperature dependence can be found, its magnitude (i.e. the coefficient) cannot be determined accurately from theory. We show that these intermediate coupling effects determine weakly temperature dependent or zero temperature quantities like the fluctuation coupling vertex or zero temperature susceptibility. These are either taken from experiment or parametrized in a simple way. The results obtained from this approach are presented in Chapters II to VI. In Chapters II and III, we compare our results with experiment for $\chi(T)$ and $C_v(T)$ of liquid He^3. The fluctuation coupling vertex is parametrized by a simple step function.

We now indicate some areas of incompleteness. In the nearly ferromagnetic regime, the specific heat has been

calculated in the quasiharmonic approximation (QHA). We have not investigated in detail the error incurred in making this approximation, i.e. the size and temperature dependence of the leading correction term. Such an estimate was made for $\chi(T)$ in Chapter II, which led to the conclusion that the fluctuation correlation corrections are small for $(T/T_F^0) = \tau \ll 1$. In the case of free energy, some simple estimates show that the diagrams left out in QHA do not contribute to leading order. However, this point needs more careful scrutiny. From experience with systems undergoing phase transitions, one finds that QHA (which translates into mean field theory) is quite good away from the critical region. Since here one is almost but never in the critical region, we expect our results to be realistic.

In the paramagnetic ($T > T_c$) regime, an important feature is the observation of spin wave like modes. These seem to be well defined for intermediate values of q, to be almost as 'stiff' as in the ferromagnetic phase for these values of q, and to become overdamped beyond a fairly sharply defined cutoff q_c. To understand this phenomenon in terms of spin fluctuations and their interactions, one has to investigate in detail the propagation of a spin triplet electron hole pair in the thermal, classical spin fluctuation field. This has been done recently by Moriya,[79] Klenin and Hertz,[80] and Ramakrishnan.[81]

We do not discuss this effect here; its influence on results obtained here for nearly ferromagnetic systems is expected to be small.

In the ferromagnetic regime, we have not made any detailed comparison between theory and experiment, either for magnetization m(T) or for spin wave stiffness D(T). The main problem is the band structure of the weak ferromagnets. Their electronic energy spectrum is not known and is perhaps not well approximated by a free electron like form. However, $m(\tau)/m(0)$ and $D(\tau)/D(0)$ curves, plotted as a function of τ for various values of τ_c, would be of value. Obtaining this requires one to solve simultaneously and selfconsistently for $m(\tau)$ and the fluctuation amplitudes $D^L(\xi_o)$, $D^T(\xi_o)$. One expects a nearly 'universal' curve because while at low temperatures $\frac{m^2(\tau)}{m^2(0)} = 1 - A\ (\frac{\tau^2}{\tau_c^2})$, at high temperatures (near τ_c) $\frac{m^2(\tau)}{m^2(0)} = (1 - B\ \frac{\tau}{\tau_c})$. A and B depend on the fermi energy. In the case of Arrott plot of $m^2(\tau)$ vs (H/m), the deviations from linearity are directly expressed in terms of $m^2(\tau)$. The deviations observed are of the right sign and show the right trend with τ; a more detailed comparison is in order. In case of $D(\tau)$, there are no data available for weak ferromagnets.

We have no satisfactory understanding of the discrepancy between the $T^{3/2}$ term present in our theory

and the $T^{5/2}$ term obtained by others for $D(T)$. An alternative way of calculating $D(T)$ is being attempted. This is basically a time dependent Ginzburg Landau (TDGL) theory, and has been used recently, for example, in discussion of dynamic critical phenomena.[82] At low temperatures there are quantum effects, i.e. fluctuations $\vec{\xi}_{\vec{q}m}$ with Matsubara frequencies $m \neq 0$ need to be considered also. Thus the usual TDGL theory, which deals with classical order parameter fluctuations, needs to be generalized. In this semiphenomenological formulation one deals directly with the equation of motion of the magnetization M in terms of functions of $\vec{M}$ and $\nabla^2\vec{M}$. The formal machinery of Chapter VI is circumvented, and the formulation is physically more direct.

Are the kind of fluctuation effects considered here important for fermi systems exhibiting other phase transitions? In the superconducting phase transition, because of the large zero temperature coherence length ξ_0, and because fluctuation coupling is sharply peaked in wave-vector and frequency space,[46] fluctuation effects are small. The BCS theory which is a generalized Hartree-Fock theory similar to that of Stoner and Wohlfarth for ferromagnetism, works quite well. In spin density wave or itinerant electron antiferromagnetic phase changes, the situation is not clear. Moriya and Hasegawa[83] have shown

that one expects considerable spin fluctuation effects. The experimental evidence can be interpreted variously, and strong band structure effects are possibly present in, say, Cr.

It is possible that the recently observed CDW phase transitions in layered chalcogenides[84,85] may afford another example where fluctuation effects of the type considered here contribute significantly to temperature dependent properties. One has, here too, an electron hole in a fermion system with strong short range coupling. Experimentally, for example, a large T^2 term in the resistivity is seen over a wide temperature range. The size is far too large to be explained by a simple Baker scattering mechanism. On the other hand, if the resistivity is due to scattering from density fluctuations with $\vec{q} \simeq \vec{Q}_{CDW}$, it is proportional to their number, which, in the low temperature range, is doubly enhanced (Chapters II and V), i.e., $n^{fluct.} \sim (T/T_{CDW})^2$. The resistivity also levels off to a nearly linear form at higher T.

APPENDIX I

In this Appendix we write the Hamiltonian of an interacting Fermi system with short range forces (zero range for simplicity) in two rotationally invariant forms. The interaction term is in the form of interacting spin and density fluctuations. Though the forms look different, a proper resummation of diagrams or perturbation series leads for example to the same RPA like criterion for ferromagnetism.

Consider the Hubbard Hamiltonian

$$H = KE + \sum_i U n_{i\uparrow} n_{i\downarrow} \tag{I.1}$$

the Stoner Hamiltonian being of course just a continuum form of I.1. We shall work with I.1; all the results obtained here are valid for the Stoner Hamiltonian too. The second term in I.1 just represents the repulsion when two fermions are on the same site. Because of the exclusion principle, they are necessarily of opposite spin. We can write

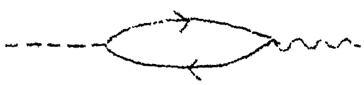
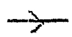
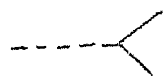
$$U n_{i\uparrow} n_{i\downarrow} = \frac{1}{2} U(n_{i\uparrow}+n_{i\downarrow}) - \frac{2}{3} \vec{S}_i \cdot \vec{S}_i \tag{I.2a}$$

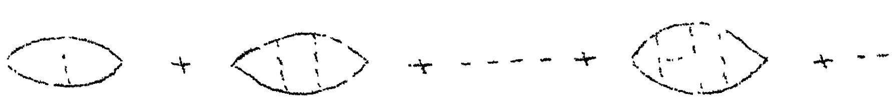
$$= \frac{1}{4} U(n_{i\uparrow}+n_{i\downarrow})^2 - \frac{1}{3} \vec{S}_i \cdot \vec{S}_i \tag{I.2b}$$

In (I.2a), except for a one body term, which can be absorbed by redifining the K.E. term, we have a quadratic form involving spin fluctuations, i.e.

$$U n_{i\uparrow} n_{i\downarrow} = \frac{1}{2} U (n_{i\uparrow} + n_{i\downarrow}) - \frac{2}{3} \sum_{\vec{q}} \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}} \qquad \text{(I.3)}$$

This rotationally invariant quadratic form is quite suitable for the functional integral transformation. This transformation is described in Chapter II, the diagrammatic rules being given in Appendix II.

It may appear from these rules and the resulting diagrams that the criterion for divergence of $\chi_{q=0}$ is $1-U'\rho_{\epsilon_F}=0$ where $U'=\frac{2U}{3}$. (We calculate the spin fluctuation propagator, with the diagram  for the self energy. Here straight lines  are electron lines and  is the bare vertex. The bare fluctuation propagator is denoted by a dotted line ------.) Thus the criterion appears to differ from the RPA. Actually one can obtain the RPA in our diagrammatic formalism with the Hamiltonian (I.3) functionally transformed. We need to sum the series



for the fluctuation self energy. This leads to the criterion

$$\left(1 - \frac{U'\rho_{\epsilon_F}}{1-\frac{U'}{2}\rho_{\epsilon_F}}\right) = 0 \quad \text{i.e.} \quad \left(1 - \frac{3U'}{2}\rho_{\epsilon_F}\right) = 0 \,. \qquad \text{(I.4)}$$

we assume that this is done, where necessary, in our work in the body of the thesis.

The form (I.2b) of $Un_{i\uparrow}n_{i\downarrow}$ is another rotationally invariant quadratic form. In this both density and spin fluctuations appear quadratically. This form is a general two body interaction, involving both spin and density fluctuations. We use this form in Chapter III, it can be used elsewhere also. Again we remark that the RPA or Stoner criterion for ferromagnetism can be obtained (after the functional transformation) by a proper resummation of diagrams for fluctuation self energy.

The variety of forms discussed above is already known for the one impurity problem (Anderson model). Keiter[91] has shown there how resummation of diagrammatic perturbation theory terms removes apparent differences. More generally, the differences are an expression of the fact that we have an intermediate coupling problem where interaction vertices cannot be determined accurately. Retaining another set of diagrams would lead to a different U_{eff} in, say the Stoner criterion.

APPENDIX II

We give here the rules for drawing various diagrams involving interaction between the fermion and the fluctuation fields. The Fourier transform of the spin density operator is defined as

$$\vec{S}_{\vec{q}} = \frac{1}{\Omega}\int d\vec{r}\; e^{-i\vec{q}.\vec{r}}\; \vec{S}(\vec{r})\,, \quad \vec{S} = \frac{1}{2}\vec{\sigma}\,,$$

so that (in the plane wave representation)

$$S^{x}_{\vec{q}} = \frac{1}{2}\left(a^{\dagger}_{\vec{k}\uparrow}\; a_{\vec{k}+\vec{q}\downarrow} + a^{\dagger}_{\vec{k}\downarrow}\; a_{\vec{k}+\vec{q}\uparrow}\right)$$

$$S^{y}_{\vec{q}} = \frac{1}{2i}\left(a^{\dagger}_{\vec{k}\uparrow}\; a_{\vec{k}+\vec{q}\downarrow} - a^{\dagger}_{\vec{k}\downarrow}\; a_{\vec{k}+\vec{q}\uparrow}\right)$$

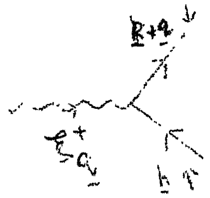
$$S^{z}_{\vec{q}} = \frac{1}{2}\left(a^{\dagger}_{\vec{k}\uparrow}\; a_{\vec{k}+\vec{q}\uparrow} - a^{\dagger}_{\vec{k}\downarrow}\; a_{\vec{k}+\vec{q}\downarrow}\right)$$

The transverse fluctuation creation operators are defined as

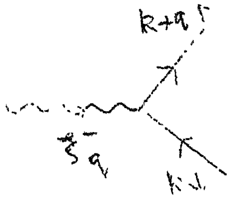
$$S^{+}_{\vec{q}} = \frac{1}{\sqrt{2}}\left(S^{x}_{\vec{q}} + i\, S^{y}_{\vec{q}}\right) = \frac{1}{\sqrt{2}}\; a^{\dagger}_{\vec{k}\uparrow}\; a_{\vec{k}+\vec{q}\downarrow}$$

and $S^{-}_{-\vec{q}} = (S^{+}_{\vec{q}})^{\dagger}$.

Now from the equation (2a.9) of Chapter II, the vertices are given by



$$:\quad 2\left(\frac{U}{\beta}\right)^{1/2} \xi^{+}_{\underline{q}}\; \frac{1}{\sqrt{2}}\; a^{\dagger}_{\vec{k}+\vec{q}\downarrow}\; a_{\vec{k}\uparrow}$$



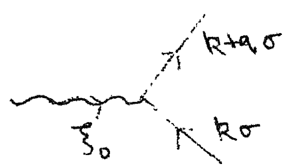
: $2\left(\frac{U}{\beta}\right)^{1/2} \xi^-_{\underline{q}} \; \frac{1}{\sqrt{2}} \; a^\dagger_{k+q\uparrow} \, a_{k\downarrow}$

: $\sigma . 2 \left(\frac{U}{\beta}\right)^{1/2} \xi^z_{qm} \; \frac{1}{2} \; a^\dagger_{k+q\sigma} \, a_{k\sigma}$

$$\sigma = + \text{ for } \uparrow$$
$$= - \text{ for } \downarrow$$

A factor of (-1) for each closed loop and a factor 1/n! for the order n of the diagram are introduced. The combinatorial factor, after considering all topologically identical diagrams, can be written as (1/S) where S is the symmetry number of the diagram (T.M.Rice, Ref. 45). A summation over all internal variables is to be performed.

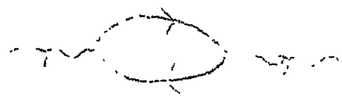
For the magnetic phase of the system, the vertex for coupling to the molecular field is



: $\sigma \; 2\left(\frac{U}{\beta}\right)^{1/2} \; \xi_o \; \frac{1}{2} \; a^\dagger_{k+q\sigma} \, a_{k\sigma}$.

The effect of the molecular field is to change the single particle energy ϵ_k to $E_k = \epsilon_k \mp (U/\beta)^{1/2} \xi_o$ and the propagator $G^o_{\underline{k}}$ to $G_{k\sigma} = (\nu_l - \epsilon_k \pm (U/\beta)^{1/2} \xi_o)$.

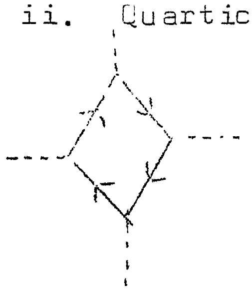
Examples:

i. RPA 

$$= (-1)\,\frac{1}{2!}\,\left(\frac{U}{\beta}\right) \sum_{\underline{k}} \left(G_{\underline{k}\uparrow}\, G_{\underline{k}+\underline{q}\uparrow} + G_{k\downarrow}\, G_{k+q\downarrow} \right)$$

$= U\chi^{0}(\underline{q})$ in the paramagnetic phase.

ii. Quartic term



$$: (-1)\,\frac{1}{4!}\, 6.2\, \left(\frac{U}{\beta}\right)^2 \sum_{\underline{k}} G_k^4 \quad \xi_0^4$$

$$= \frac{-1}{2}\,\frac{U_4}{\beta U}\,. \quad \xi_o{}^4\,.$$

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